COM-MAT-FAIL

Computational Material Failure

User Guide

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Introduction

The preliminary purpose of this document is to aid `commatfail` users and developers in getting some basic tools when using the code for themselves. It was conceived after the research work of many people, and as the final work to stop the implementation of new features in this code. It can not be viewed neither as a rigorous manual nor an exhaustive description of each line in the code.

Readers who are a only user of the code, and are not interested in the implementation of new features, should probably go to read only chapter 2 and 3. Those chapters will guide the user through the rules to keep in mind when writing or creating an input file. For developers, we recommend a careful reading of the entire document, so they have a better idea of how the code is structured.

Pre-requisites

The `commatfail` users do not require to have additional software in their machines. Executable binaries are already compiled for Windows platform, and should be used in a command line prompt.

The `commatfail` developers should have installed Microsoft Visual Studio 2010, and Intel Visual Fortran Composer 2011. Other IDEs compilers are not recommended for a correct functionality of the code.

Installation

There is no need to install `commatfail`. If the pre-requisites are met, the solution file `commatfail.sln` should open in Microsoft Visual Studio with no problems.

Running `commatfail` and `commatfailpost`

Binaries and input file should be in the same working directory. Computations should be done in a command line prompt with:

```
commatfail <input_file_name>
```

If GiD will be used to see the results, post-process should be done after computations in a command line prompt with:

```
commatfailpost <input_file_name>
```

After post-process, results can be seen opening the file "`<input_file_name>_s1.flavia`" in GiD pre/post processor.

Clarity of the code

Finite element codes are no exception when facing the dilemma of clarity versus efficiency. Even though those are not opposite concepts, an effort to achieve one tends to lack the other. The

programming philosophy adopted in the development of commatfail has been the optimization of procedures. This does not mean that the creators of the code have done their best to make it as comprehensible as possible.

Portability

Most commatfail routines are written in a standard Fortran 90 programming language, but some small details are only valid for Intel Fortran Compiler. Currently the code is already configured in a Microsoft Visual Basic 2010 solution, and its usage with other compilers and IDE's could need some extra configurations for its correct operation.

General convention for character fonts

The meaning associated to specific font styles is given below. Standard typos are not explained here, and some exceptions could be highlighted in the text and not here.

Description	Example
Scalar values and functions	a, α, A
Vectors	$\boldsymbol{a}$, $\boldsymbol{n}$
Second order tensors	$\boldsymbol{B}$, $\boldsymbol{\sigma}$
Forth order tensors	$\mathbf{C}$, $\mathbf{S}$
Spaces	$\mathcal{U}$, $\mathcal{V}$
Fortran codes, plain text, file names	`<input>.dat`, `NEW_MATERIAL`
Key or button pressing indications	Apply, esc
Software menus	***File*** $>$ ***Save as***, ***Data*** $>$ ***Problem data***

Chapter 1

Overview of commatfail

commatfail is a multipurpose finite element code written in Fortran 90. As many finite element codes, it has only the calculus process of a problem. That means that all needed information is taken from an input file before the computations start, and all results are written in the output files when finished. Figure 1.1 shows this basic way of how commatfail works[1].

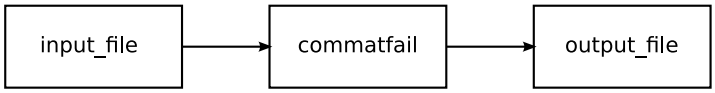


Figure 1.1: commatfail basic operating process

To perform a simulations with commatfail:

1. Place the input file and the executable commatfail file in the same directory.
2. Navigate to that directory through a command window.
3. Execute: commatfail <input_file>

After the calculations are done, post-process can be done by:

1. Place the executable file commatfailpost in the same directory.
2. Execute in the command window: commatfailpost <input_file>

The user could write a simple script to execute those commands more efficiently, especially when more than one simulation is to be done sequentially.

1.1 Modules and database

Once the input file is supplied, there are some subroutines in commatfail which reads all the problem data, and create a temporary database to check whether all required fields are complete. If so, an internal database is created to be used later while the calculations are done. This database is stored in modules[2], and its main role is to communicate among the calculation subroutines and keep the variables in one place.

These modules can be found in the files whose name ends with *_db.f90. Some of those modules are:

- elmset_db.f90: stores the information on element sets.

[1] Note that the input and output files should be generated and read with some external software capable of pre-process and post-process a finite element problem.

[2] This implies that variables are global and not local. This brings advantages, e.g. not use many variables as input and output arguments in all subroutines

- nodeset_db.f90: stores the information on nodes, as the coordinates.
- mat_db.f90: stores the information of materials properties.

1.2 Stages

A simulation in commatfail can be done by *stages*, which may have different conditions of loads or element properties. Suppose that we

The type of stages allowed are:

- NEW_PROBLEM
- NEW_STAGE
- RESTART_STAGE
- RESTART_CALC
- RESTART_NEWMSH

1.3 The main program

The main commatfail procedure is done by mainpg. It can be divided into three basic parts:

1. *Initialization and input data.* The initialization of the execution parameters is carried out in this phase, at the very beginning of the execution of the program. The reading precess of the input data is done at the beginning of each stage from the input data text file or the restart file.
2. *The incremental finite element procedure.* This is the main body of the program, where all the numerical calculations associated to the finite element method are done. This procedure is done one time for each stage of the problem, after reading the input data. Essentially it consist of a time-steps integration process with an interface routine (calcstg) that chooses the calculation method depending on the integration scheme: implicit, explicit, or implicit-explicit.

   This comprises all output operations necessary to print converged finite element solutions into the results file and/or dump an image of the database into a restart output file. Output routines are called from inside the main loop over load increments.
3. *Write output results.* This comprises all output operations necessary to print converged finite element solutions into the results or restart files.Those routines write in files with the correct format to be read with the post-processor commatfailpost. Output files from commatfailpost are then in the correct format to be imported in GiD.

1.4 Description of files managed by commatfail

commatfail manages the opening and closing of files through two routines. The routine that handles the opening of files is called "openfi" while the routine that manages the closing of files is called "closefi". In turn, both depend on a common module called "filevar_db" in which units and extensions are defined. The manipulation of files at the programming level required to make co-ordinated development of this module and these two routines.

- commatfail.dat: This file actually corresponds to the data file that will be used by the program and it is a single file with normal ASCII characters. One of the first tasks of commatfail when launching a new calculation is to build this file from the data files provided by the user. In case the data file provided by the user is unique, commatfail.dat is a copy of it.

- <name>.scr: A type of report file that replicates all the information that comes to the screen.
- <name>.rpt: A type of report file that provides basic information such as command line launched, if the calculation is new or a restart, start date and time of release, number of elements for the problem, and real time calculation of CPU, etc. and it is useful for a novice user.
- <name>.rsn: A type of file focused on advanced or very advanced user. It includes all information to be introduced to monitor the tasks performed by the code. You may have even intended to be used in debug mode.
- <name>.rsf: An internal file in commatfail to save all the information necessary to relaunch the calculation either by an unwanted interruption of the program or to launch a new phase or stage.
- <name>.sun: It is a binary file that contains all the results of post-processing problem in the form of commatfail, which must then be interpreted by the module commatfailpost.
- <name>.nlb: It is an ASCII file that contains, for each stage, all the changes to the labels of the nodes that overlap with other nodes automatically added by commatfail or added by the user in previous stages.
- <name>.c01, <name>.c02, etc.: They are text files that contain all data for plotting the plots defined in the input file.
- <name>_s1.flavia: This is a binary file that contains all the results in the correct format to be read by pre/post-process tool GiD. It should be open from GiD.

Rules. *Although the operating system allows it, commatfail does not allow path or file names contain spaces.*

1.5 File commands

- ImportFile = <file_name>

Rules. *The command ImportFile can be located anywhere in the data file. However, it must be the only command line.*

One of the first tasks undertaken by commatfail is to interpret the file or data file provided by the user and make a copy from them in an auxiliary data file called "commatfail.dat". The auxiliary data file is unique (a single file) and this is the file that commatfail reads during implementation. However, this is a temporary file to be deleted automatically after the execution of commatfail.

1.6 Code comments

commatfail allows you to enter any comments deemed necessary in order to help or clarify or interpret the data file. However, comments will be given by the program. The comments in the data file are marked by the characters "!" Or "#".

Rules. *The character "#" should be located in the first column which indicates the program that the entire row is a comment.*

The character "!" can be located anywhere on the line after any command, telling the program from that position until the final line is a comment.

Obviously, the character "!" can also be located in the first column to perform the same functions as the "#" character, so this is a more general command.

Chapter 2

Input data file for commatfail

2.1 Creating input data file

BEGIN_PROBLEM and END_PROBLEM identify, respectively, the beginning and the end of the actual data file.

```
BEGIN_PROBLEM
  <problem body data>
END_PROBLEM
```

- BEGIN_PROBLEM: is the keyword to specify the beginning of the actual data file.
- END_PROBLEM: is the keyword to indicate the ending of the actual data file.

Rules. *The definition of this field is mandatory in every data file. It is the field that encompasses all other fields in the data file that can be defined and interpreted by the program. However, it only allows defining a single data input field.*

This field may contain general commands such as the import file (ImportFile), the title of the problem (Begin_Problem_Basics or End_Problem_basics) or the definition of stages (New_Stage or End_New_Stage). Any command outside this field is not interpreted by the program.

Example

```
BEGIN_PROBLEM
  BEGIN_PROBLEM_BASICS
    ...
  END_PROBLEM_BASICS
  NEW_STAGE
    ...
  END_NEW_STAGE
END_PROBLEM
```

2.2 Creating the problem basics

BEGIN_PROBLEM_BASICS and END_PROBLEM_BASICS are the key words that identify the beginning and the end, respectively, of the general data of the problem such as the name (title) of the problem, size or the default time integration scheme, the solver and the tolerance of the stages.

```
BEGIN_PROBLEM_BASICS
  TITLE = <Problem Title>
  SCRLEVEL = <number>
  RSNLEVEL = <number>
  NDIME = <Problem Dimension>
  STAGE_TYPE = <Type of stage>
```

```
  SOLVER_TYPE = <Solver Type>
  MAX_ITERATION = <Max. no. of iterations per time step>
  TOLERANCE = <Convergence tolerance>
  MESH_POST = Option <YES / NO>
END_PROBLEM_BASICS
```

- BEGIN_PROBLEM_BASICS: is the command or keyword that identifies the beginning of the field.
- END_PROBLEM: is the command or keyword that identifies the end of the field.
- TITLE: is the command or keyword used to indicate the title of the problem described by the data file. Must be preceded by a string or sentence.
- SCRLEVEL: is the command or keyword used to indicate the level of messages going to be appeared on screen and in the *.scr file. This command must be preceded by a positive integer that indicates the level of messages per screen (the higher the number the greater number of messages will appear). By default the value is considered 0.
- RSNLEVEL: is the command or keyword used to indicate the level of messages in the file *.rsn. This command must be preceded by a positive integer that indicates the level of messages per screen (the higher the number the greater number of messages will appear). By default the value is considered 0.
- NDIME: is the command or keyword used to indicate the dimension of the problem. This command must be preceded by a positive integer that indicates the dimension of the problem: 1 to 1D problems (there are currently no scheduled element for 1D), 2 and 3 for 2D problems and for 3D problems.
- STAGE_TYPE: is the command or keyword to indicate the type of stage (e.g. an incremental integration scheme in time implied a re-accommodation or body) and should be preceded by a keyword predefined by the program according to the types of stages that has been implemented. Currently, the program takes into consideration the following:
  - IMPLICIT_NR: implicit integration scheme using Newton-Raphson scheme.
  - IMPLICIT_NR_V2: implicit integration scheme using Newton-Raphson scheme similar to the preceding but which converges in one step if the problem is linear (default option).
  - EXPLICIT: explicit integration scheme (not scheduled yet).
  - BODY_MOVE: rearranging or moving solid rigid bodies (not scheduled yet).

  The default option "IMPLICIT_NR" is assigned when this command is not explicitly stated in some of the stages. However, the obligation of the command depends on the type of SOLVER_TYPE.
- SOLVER_TYPE: is the command or keyword to indicate the type of solver to be used and should be preceded by a keyword predefined by the program according to the type of solver that has already been implemented. Currently, the program takes into consideration the following solvers:
  - GAUSSJORDAN: direct solver by Gauss-Jordan elimination with full matrix. Use of this solver is limited, for smaller examples.
  - LU: direct solver with full storage array. Use of this solver is not meant to medium/large problems, so its use is limited only to debug small examples.
  - SUPERLU: direct solver with storage of the sparse matrix type. This constraint solver has the ability to contain the decomposition of the matrix in memory.

- MAX_ITERATION: is the command or keyword to specify the value for the maximum number of iterations required for convergence per time step and must be preceded by a whole number.
- TOLERANCE: is the command or keyword to specify the value of tolerance required for convergence and it must be preceded by a real number.
- MESH_POST: is the command or keyword to specify the option of post process for different stage. If the option is YES the results will be post-processed for all meshes although these results are not partners. If the option is NO, only post-processed mesh containing those results, in which case it overwrites the filenames that are not associated any results. The default option is NO.

  Rules. *This is a mandatory field whose absence will create an error that will stop the program. This statement is made in the data input field (if stated in a different field will cause an error) and can be located anywhere in the field although it is recommended to write at the beginning. It can contain any command on the general variables of the problem and any command outside this field will not be interpreted as Problem Basics.*

  Problem Basics no one field to another field may contain either one Problem Basics Field Stage.

- SCRLEVEL: the command is optional and can be located anywhere in the field Problem Basics, although it is recommended to be in the starting of the field. The declared value in this field will be valid for the whole problem, unless otherwise explicitly specified in a Stage (see Creation Basics Field Stage). The whole number into SCRLEVEL indicates the level of messages you want to get in the screen. The lowest integer is 0 and there is no upper limit. The higher the level the greater the number of messages per screen. Thus, if the level is 0 during the execution minimum number of messages will be written.
- RSNLEVEL: the command is optional and can be located anywhere in the field Problem Basics. The declared value in this field will be valid for the whole problem, unless explicitly specified in a Stage (see Creation Basics Field Stage). The whole number into RSNLEVEL indicates the level of messages you want to get in the file *.rsn. The lowest integer is 0 and there is no upper limit for it. The higher the level the greater the number of messages sent to the file *.rsn. Thus, if the level is 0 during the execution minimum number of messages will be written.
- NDIME: this command is required.

Example

```
BEGIN_PROBLEM BASICS
  TITLE = 5061 piece with a sequence of three movements
  SCRLEVEL = 1
  RSNLEVEL = 1
  NDIME = 2
  STAGE_TYPE = IMPLICIT_NR
  SOLVER = SuperLU
  MAX_ITERATION = 100
  TOLERANCE = 1d-6
END_PROBLEM_BASICS
```

2.3 Creating the stage

NEW_STAGE and END_NEW_STAGE are the key words that identify the beginning and the end of the field respectively with the data describing the Stage.

```
NEW_STAGE
  <Stage body data>
END_NEW_STAGE
```

- NEW_STAGE is the command or keyword used to indicate the beginning of the field.
- END_NEW_STAGE is the command or keyword used to indicate the end of the field.

Rules. *This field can contain any command. Any command on the information of Stage located outside the field will not be interpreted as a figure of the Stage.*

A transaction may not contain field to another field Stage. However, it can contain other fields such as field Stage Basics, Material field, Section field, the Set of Elements field, etc.

Example

```
NEW_STAGE
  BEGIN_STAGE_BASICS
  ...
  END_STAGE_BASICS
  BEGIN_MATERIAL
  ...
  END_MATERIAL
END_NEW_STAGE
```

2.4 Creating the stage basics

BEGIN_STAGE_BASICS and END_STAGE_BASICS are the key words that identify the beginning and the end respectively of the general data of a stage as it includes information on stage name, size or time integration scheme, the solver, the tolerance, the number of increments or the time of completion of the stage.

```
BEGIN_STAGE_BASICS
  TITLE = <Title of the stage>
  SCRLEVEL = <enter number>
  RSNLEVEL = < enter number >
  STAGE_TYPE = <Type of stage>
  SOLVER_TYPE = <Type of solver>
  MAX_ITERATION = <Max no. of iterations per step>
  TOLERANCE = <tolerance of convergence>
  NUMBER_STEPS = <No. of increments of the stage>
  NUMBER_POST = <No. of steps for post-processing>
  PERIOD_POST = <time period for post-processing >
  END_TIME = <final time of the stage>
  DYNAMIC_TYPE = <Type of dynamic integration>
  MESH_POST = <YES / NO>
END_STAGE_BASICS
```

- BEGIN_STAGE_BASICS: is the command or keyword that identifies the beginning of the field.
- END_STAGE_BASICS: is the command or keyword that identifies the end of the field.
- TITLE: is the command or keyword used to indicate the title of the stage. Must be preceded by a string or sentence.
- SCRLEVEL: is the command or keyword used to indicate the level of messages on screen and in the *.scr file in the stage. This command must be preceded by a positive integer that indicates the level of messages per screen (the higher the value the greater number of messages). By default the value is considered 0.

- RSNLEVEL: is the command or keyword used to indicate the level of messages in the file *.rsn during the stage. This command must be preceded by a positive integer that indicates the level of messages per screen (the higher the value the greater number of messages). By default the value is considered 0.

- STAGE_TYPE: is the command or keyword to indicate the type of stage and should be preceded by a keyword predefined by the program according to the types of Stages implemented. Currently, the program takes into consideration the following:

  - IMPLICIT_NR: implicit integration scheme using Newton-Raphson scheme.
  - IMPLICIT_NR_V2: implicit integration scheme using Newton-Raphson scheme similar to the preceding but which converges in one step if the problem linear (default option).
  - EXPLICIT: explicit integration scheme (not implemented yet).
  - BODY_MOVE: rearranging or moving solid rigid bodies (not implemented yet).

- SOLVER_TYPE: is the command or keyword to indicate the type of Solver to use during the stage and must be preceded by a keyword predefined by the program according to the type of solver implemented (see "Problem basics").

- MAX_ITERATION: is the command or keyword to specify the value for the maximum number of iterations for convergence for the stage and should be preceded by a whole number.

- TOLERANCE: is the command or keyword to specify the value of convergence tolerance for the stage and should be preceded by a real number.

- NUMBER_STEPS: is the command or keyword used to indicate the number of increments or time steps for the stage. This command must be preceded by a positive integer indicating the number of increments.

- NUMBER_POST: is the command or keyword used to indicate the number of post-processing carried out on the stage following a long constant frequency. This command must be preceded by a positive integer indicating the number of increments.

- PERIOD_POST: is the command or keyword used to indicate the frequency of post-processing carried out on the stage by defining the time period. This command must be preceded by a positive real number indicating the number of increments.

- END_TIME: is the command or keyword to specify the value of the final moment of the stage and should be preceded by a real number.

- DYNAMIC_TYPE: is the command or keyword used to indicate the type of dynamic integration to be used for the stage and should be preceded by a keyword. Currently, the code supports the dynamic integration:

  - STATIC: Keyword to specify a static calculation (default option). Requires no additional parameters.
  - G_ALPHA: Keyword to specify a dynamic calculation using the general Alpha-method. This method requires the definition of additional parameters.

- MESH_POST: is the command or keyword to specify the option type in the post-processing stage. If the option is YES is post-processed all meshes although these results are not partners. If the option is NO only post-processed mesh containing those results, in which case it overwrites the filenames that are not associated any results.

- BEGIN_DYNAMIC_PARAMETERS: keyword which opens the field to interpret the parameters of the dynamic integration.

- END_DYNAMIC_PARAMETERS: keyword closing the field which is used to interpret the parameters of the dynamic integration.

Rules. *The field of STAGE_BASICS is declared within a Stage Field (if declared in a different field will cause an error) and can be located anywhere in the field although it is strongly recommended that it is the first stage of the field or in case some messages may be lost during reading. It can contain any command of general variables and any command on this field, if written outside this field will not be interpreted as Stage Basics.*

No other field can contain Stage Basics. However, when a new stage is set (NEW_STAGE - END_NEW_STAGE) it is necessary to define a field as STAGE_BASICS which defines the characteristics of the new stage.

The command SCRLEVEL is optional and can be located anywhere in the Stage Basics field, however it is strongly recommended to write it in the beginning or otherwise some messages might be lost during reading. The declared value in this field will overwrite the value that was defined in the Problem Basics (see Problem Basics). The whole number into SCRLEVEL indicates the level of messages you want to get in the screen. The lowest integer is 0 and says there is no upper limit. The higher the level the greater the number of messages per screen. Thus, if the level is 0 during the execution only the minimum number of messages will be written.

*The command RSNLEVEL is optional and can be located anywhere in the Stage Basics field, however it is strongly recommended to write it in the beginning or otherwise some messages might be lost during the reading. The declared value in this field will overlap the value that was defined in the Problem Basics (see field Problem Basics). The whole number into RSNLEVEL indicates the level of messages you want to get into the file *.rsn. The lowest integer is 0 and says there is no upper limit. The higher the level the greater the number of messages sent to the file *.rsn Thus, if the level is 0 during the execution only the minimum number of messages will be written.*

The command STAGE_TYPE is mandatory if it has not been declared in the Problem Basics. However, compulsory SOLVER_TYPE command depends on the integration scheme employed.

Commands such as NUMBER_STEPS, NUMBER_POST, PERIOD_POST and END_TIME are unique to the stage.

Commands NUMBER_POST and PERIOD_POST are optional and mutually exclusive. In case both are set simultaneously, the information defined by the command NUMBER_POST precedes over that defined by the command PERIOD_POST. In the event that the stage does not define any of these commands, only the final stage will be post-processed.

Example

```
BEGIN_STAGE_BASICS
  TITLE = Stage pressing - First movement of punches
  SCRLEVEL = 3
  RSNLEVEL = 3
  SOLVER = SuperLU
  MAX_ITERATION = 100
  TOLERANCE = 1d-3
  NUMBER_STEPS = 100
  NUMBER_POST = 3
  End_time = 1d-2
END_STAGE_BASICS
```

2.5 Creating the material data base

BEGIN_MATERIAL and END_MATERIAL are, respectively, the key words that identify the beginning and the end of the materials database.

```
BEGIN_MATERIAL
  DELETE = <label of the material>
```

```
  NEW_MATERIAL
    <body defining new material data>
  END_NEW_MATERIAL
END_MATERIAL
```

- BEGIN_MATERIAL: is the keyword indicating the starting of the material data.
- END_MATERIAL: is the key word to indicate the end of the material data.
- DELETE: This is the keyword to specify the name of material (label) to be removed from the database of material. Must be preceded by the label for the material to be removed.
- NEW_MATERIAL: Keyword which opens the data field that defines a material database (see scope of materials).
- END_NEW_MATERIAL: Key word which closes the field with the data that define a material database (see scope of materials).

Rules. *This field allows you to communicate with the database of materials used in the calculation, creating and removing the materials from the database. The following commands may be repeated as necessary: DELETE, NEW_MATERIAL and END_NEW_MATERIAL.*

Example

```
BEGIN_MATERIAL
  DELETE = material_1
  DELETE = material_2

  NEW_MATERIAL
    ...
  END_NEW_MATERIAL

  NEW_MATERIAL
    ...
  END_NEW_MATERIAL
END_MATERIAL
```

2.6 Creating the material properties

NEW_MATERIAL and END_NEW_MATERIAL are, respectively, the key words that identify the beginning and the end of the data set that defines a material.

```
NEW_MATERIAL
  NAME = <material label>
  TYPE = <type of_material>
  NEW_SUBMATERIAL
    <properties of the material>
  END_NEW_SUBMATERIAL
END_NEW_MATERIAL
```

- NEW_MATERIAL: is the keyword that indicates the beginning of the data that characterize the material.
- END_NEW_MATERIAL: is the keyword that indicates the end of the data that characterize the material.

- NAME: is the keyword to specify the name of material (label) that will identify the database and must be preceded by a word that will gain the category label. It is a mandatory parameter and is recommended to be located at the beginning of the field.
- TYPE: is the keyword to specify the type of material (if material is a standard or defined by the user, etc.) and must be preceded by a keyword predefined by the program according to the type of material. It is a mandatory parameter and must be located at the beginning of the field before the definition of submaterials.
- NEW_SUBMATERIAL: Keyword which opens the field of sub-material, which defines at least a portion of the material characteristics such as the elastic model, the surface creep, and so on. (see submaterials field).
- END_NEW_SUBMATERIAL: Keyword which closes the sub-material field.

Rules. *This field can contain any command or data on the parameters of the material, and any information on the material located outside the field shall not be interpreted.*

It is mandatory to define a label identifying the material, which is achieved through the NAME command in this field. Failure generates an error in reading inputs that will stop the program.

To define the material properties one can define as many sub-fields of material as needed.

It is mandatory to define the type of material before the submaterials, which is achieved through the TYPE command at the beginning of this field. Omission of this or statement after submaterial generates an error in reading inputs that will stop the program.

Example

```
NEW_MATERIAL
  NAME = material_1
  TYPE = ELASTOPLASTIC
  NEW_SUBMATERIAL
    ...
  END_NEW_SUBMATERIAL
END_NEW_MATERIAL
```

2.7 Creating the sub-material properties

NEW_SUBMATERIAL and END_NEW_SUBMATERIAL are, respectively, the key words that identify the beginning and the end of the data set that defines the characteristics of the material or the submodel (e.g. the elastic model, the surface creep, hardening laws, etc).

```
NEW_SUBMATERIAL
  NAME = <label of_sub-material>
  TYPE = <type of_sub-material>
  BEGIN_PARAMETERS
    <properties of the sub-material>
  END_PARAMETERS
  NEW_CURVE
    <curves that define the points of the sub-material>
  END_NEW_CURVE
  NEW_SUBMATERIAL
    <defining nested sub-material>
  END_NEW_SUBMATERIAL
END_NEW_SUBMATERIAL
```

- NEW_SUBMATERIAL: is the keyword that indicates the beginning of the data that characterize the sub-material. If this keyword is declared within the field itself, it implies declaring another submodel of material nested in the actual submodel.

- END_NEW_SUBMATERIAL: is the keyword that indicates the end of the data that characterize the sub-material. If there is another submodel within the stated submodel, then this keyword closes the later field.

- NAME: is the keyword to specify the name of the material submodel (label) that will identify the sub-material. Must be preceded by a word that will gain the category label. It is a mandatory parameter and is recommended to be located at the beginning of the field.

- TYPE: is the keyword to specify the type of submodel (linear elastic, elastoplastic, etc.), and must be preceded by a keyword predefined by the program according to the type of material submodel. It is a mandatory parameter and is recommended to be located at the beginning of the field with the only restriction to be observed that it comes before the command BEGIN_PARAMETERS.

- BEGIN_PARAMETERS: Keyword which opens the field to interpret the constants that define the submodel of material such as elastic model, surface creep, and so on.

- END_PARAMETERS: Key word which declares the closing of the field of material parameters for the submodel.

- NEW_CURVE: Keyword that paves the way to interpret a curve (see Definition field curves).

- END_NEW_CURVE: Key word which declares the closing of the field of material curves.

Rules. *This field can contain any command or data on the parameters of submodel, and any material information located outside shall not be interpreted.*

It is mandatory to define a label identifying the material, which is achieved through the NAME command in this field. Failure generates an error in reading inputs that will stop the program. It is also mandatory to define the type of submodel through the TYPE command, the omission of which also generates a reading error that stops the execution.

To define the properties of the submodel, it is defined by a single field parameter (BEGIN_PARAMETERS and END_PARAMETERS), but you can define as many fields as necessary curves to define the submodel material.

It is allowed that a submodel of material can be composed of different submodels of material so that the base material is dynamic and flexible.

Example

```
NEW_SUBMATERIAL
  NAME = model_elastic_1
  TYPE = ELASTIC_LINEAR
  BEGIN_PARAMETERS
    YOUNG = 2.1E +6
    POISSON = 0.29
  END_PARAMETERS
  NEW_CURVE
    ...
  END_NEW_CURVE
END_NEW_SUBMATERIAL
```

2.8 Defining curves

NEW_CURVE and END_NEW_CURVE are the key words that identify the beginning and the end respectively of the data set that define a curve, which may be defined by a cloud of points or any other data set and define the interpretation of which is scheduled.

```
NEW_CURVE
  NAME = <label of the curve>
  TYPE = <type of curve>
  BEGIN_PARAMETERS
    <body hat defines the curve>
  END_PARAMETERS
END_NEW_CURVE
```

- NEW_CURVE: is the keyword that indicates the beginning of the data that characterizes the curve.
- END_NEW_CURVE: is the keyword that indicates the end of the data that characterizes the curve.
- NAME: is the keyword to specify the name of the curve (label) that will identify the rest of the curves defined on the basis of corresponding curves. Must be preceded by a word that will gain the category label. It is a mandatory parameter and is recommended to be located at the beginning of the field.
- TYPE: is the keyword to specify the type of the curve (if a cloud of points or any other family of curves that is scheduled) and should be preceded by a keyword predefined by the program according to the type of curve. It is a mandatory parameter and is recommended to be located at the beginning of the field with the only restriction to be observed that it comes before the field BEGIN_PARAMETERS. Currently, the program takes into consideration the following types:
  - BY_POINTS: curve defined by points.
- BEGIN_PARAMETERS: Keyword that paves the way to interpret the data that define the curve.
- END_PARAMETERS: Key word that closes the field of parameters that define the curve.

Rules. *This field can contain any command or data on the curves and any command or data outside of it will not be interpreted.*

It is mandatory to define a label that identifies and distinguishes the rest of the curve, which is achieved through the NAME command in this field. Failure generates an error in input reading that stops the program. Furthermore, the label of the curve is restricted to the set of curves defined by the base curve. Two different materials, for example, can have separate curves with identical labels and there is no conflict because the discrimination between the two is done via the label on the material and therefore are two different base curves.

It is also mandatory to define the type of curve through the TYPE command, the omission of which also generates a reading error that stops the execution.

The data of the curve are introduced in a single field parameter (BEGIN_PARAMETERS and END_PARAMETERS).

Example

```
NEW_CURVE
  NAME = curve_1
  TYPE = BY_POINTS
  BEGIN_PARAMETERS
    ! --- Curve defined by 3 points
    0.0 0.0
    1.0 20.0
    2.0 -20.0
  END_PARAMETERS
END_NEW_CURVE
```

2.9 Establishment of the basis of sections

BEGIN_SECTION and END_SECTION are the key words that identify the beginning and end of all the additional data associated with the element (including the reference material) and are not directly related to the geometric definition of the mesh.

```
BEGIN_SECTION
  DELETE = <section label>
  ASSOCIATE: SECTION = <section label> MATERIAL = <material label>
  NEW_SECTION
    <body that defines all or part of the base sections>
  END_NEW_SECTION
END_SECTION
```

- BEGIN_SECTION: is the keyword that indicates the beginning of the data for the sections.
- END_SECTION: is the keyword that indicates the end of the data for the sections.
- DELETE: This is the keyword to specify the section name (label) to be removed from the database. Must be preceded by the label of the section to remove.
- ASSOCIATE: is the keyword to specify the link to the material section. This option must be accompanied by keywords:
  - SECTION: followed by the label of the section to associate.
  - MATERIAL: followed by the material label that is associated with the section.
- NEW_SECTION: Keyword which opens the field with data that defines a section of the database.
- END_NEW_SECTION: Key word here closes the field with data that defines a section of the database.

Rules. *This field allows you to communicate with the Section database containing data associated with the element type (e.g. material associated with an element of the mesh, if the problem is a two-dimensional plane strain, etc.). The following commands may be repeated as necessary: such as: DELETE, NEW_SECTION and END_NEW_SECTION.*

ASSOCIATE option should be used when the material associated with the section is removed and then re-created. In these circumstances, the association of the section breaks at the time when the material is removed; it is necessary to re-link the material for the purpose of the program and is considered as a new material.

Example

```
BEGIN_SECTION
  DELETE = section_1
  DELETE = section_2
  ASSOCIATE: SECTION = section_1 MATERIAL = material_1
  NEW_SECTION
    ...
  END_NEW_SECTION
  NEW_SECTION
    ...
  END_NEW_SECTION
END_SECTION
```

2.10 Creating the sections

NEW_SECTION and END_NEW_SECTION are the key words that identify the beginning and end respectively of the data set associated with each of the sections involved in the mesh (for example, if a body is composed of two materials, it would have at least two sections each one of which would be associated respectively with the elements of the mesh and with the material they are made).

```
NEW_SECTION
  NAME = <section label>
  TYPE = <type of section>
  BEGIN_PARAMETERS
  MATERIAL = <associated material label>
    <body that define the properties of section>
  END_PARAMETERS
END_NEW_SECTION
```

- NEW_SECTION: is the keyword that indicates the beginning of the data that characterize the section.
- END_NEW_SECTION: is the keyword that indicates the end of the data that characterize the section.
- NAME: is the keyword to specify the section name (label) that will identify in the database of the sections. Must be preceded by a word that will gain the category label. It is a mandatory parameter and is recommended to be located at the beginning of the field.
- TYPE: is the keyword to specify the type of section, and therefore that data is needed and should be interpreted. Must be preceded by a keyword predefined by the program according to the type of section. It is a mandatory parameter and is recommended to be located at the beginning of the field with the only restriction to be observed that it is before the field BEGIN_PARAMETERS. Currently, the code has the following options:
  - MATERIAL_SECTION: Elements: 3D elements in general and that they only need to associate a material.
  - PLANE_STRAIN: Elements 2D plane strain problems.
  - PLANE_STRESS: Elements 2D plane strain problems.
  - AXISIMMETRIC: Elements 2D axisymmetric problems.
- BEGIN_PARAMETERS: Keyword that paves the way to interpret the data that define the section such as the material to which it is associated, and so on.
- END_PARAMETERS: Keyword closing the field used to describe the parameters that define the section.

Rules. *This field can contain any command or data on the sections and any command or data located outside shall not be interpreted in relation to the database of the sections.*

It is mandatory to define a label that identifies the section, which is achieved through the NAME command in this field. Failure generates an error in input reading that will stop the program.

It is also mandatory to define the type of section through the TYPE command, the omission of which also generates a read error that stops the execution.

The section data is introduced into a single field parameter (BEGIN_PARAMETERS and END_PARAMETERS).

Example

```
NEW_SECTION
  NAME = section_1
  TYPE = PLANE_STRESS
```

```
  BEGIN_PARAMETERS
    MATERIAL = AL4030
    THICK = 1.0E-3
  END_PARAMETERS
END_NEW_SECTION
```

2.11 Establishment of the basis of nodes

BEGIN_NODE_SET and END_NODE_SET are the key words that identify the beginning and end respectively of the data set (node labels and their coordinates) associated with the set of nodes.

```
BEGIN_NODE_SET
  DELETE_SET = <node set label>
  DELETE_SUBSET = <node subset label>
  NEW_NODE_SET
    <body that defines the set of nodes>
  END_NEW_NODE_SET
  NEW_NODE_SUBSET
    <body that defines the subset of nodes>
  END_NEW_NODE_SUBSET
END_NODE_SET
```

- BEGIN_NODE_SET: is the keyword that indicates the beginning of the data for the node.
- END_NODE_SET: is the keyword that indicates the end of the data for the node.
- DELETE_SET: is the keyword to specify the name of the set of nodes (label) to be removed from the database. Must be preceded by the label for the set of nodes to remove.
- DELETE_SUBSET: is the keyword to specify the name of the subset of nodes (label) to be removed from the database. Must be preceded by the label for the subset of nodes to remove.
- NEW_NODE_SET: Keyword which opens the field of the data that define a set of nodes in the database (see section Creating the "Node Set").
- END_NEW_NODE_SET: Key word here closes the field with the data that define a set of nodes in the database (see section Creating the "Node Set").
- NEW_NODE_SUBSET: Keyword which opens the field with the data defining a grouping of nodes in the database (see section Creating the "Subset of Nodes").
- END_NEW_NODE_SUBSET: Key word here closes the field with the data defining a grouping of nodes in the database (see section Creating the "Subset of Nodes").

Rules. *This field allows you to communicate with the database of Set of nodes that contain data associated with nodes (tags and coordinates). The commands such as, DELETE_SET or NEW_NODE_SET and END_NEW_NODE_SET may be repeated as necessary.*

The set of nodes should be interpreted as how to declare the program all nodes involved in the problem. This statement should be made for at least one set of nodes that may be unique regardless of the type of problem. However, this statement can subdivide the set of nodes in a number of sets, for the sake of clarity (e.g. a set of nodes for each body that composes the problem).

It is mandatory that the nodes are declared through a set of nodes, but a node can not belong simultaneously in two or more different sets of nodes.

If a calculation for adding new nodes after remeshing is produced, it is possible to change the labels of the nodes added when they come into conflict with the labels of nodes generated during remeshing. In this case, all references to the nodes in the corresponding stage (like the table of

connectivities, degrees of freedom of a node, etc) are considered for the new added nodes whose labels have been corrected.

This field also allows communication with the database Subset of Nodes that contain data associated with any particular group of nodes (identified only by their labels). This may be repeated as necessary with the commands DELETE_SUBSET or NEW_NODE_SUBSET and END_NEW_NODE_SUBSET.

The subset of nodes to be interpreted as ways of defining groups of nodes. This is especially useful when these nodes share a common property which is referenced throughout instead of a group (e.g. a set of nodes that have the same displacement).

When a subset of nodes is cleared during a stage with the command DELETE_SUBSET, then during this stage it can not generate a subset of nodes with the same name as the deleted one. It avoids ambiguities in interpreting the subset of nodes.

The nodes can belong to several subsets of nodes (subset) or none.

Example

```
BEGIN_NODE_SET
  DELETE_SET = node_set_1
  NEW_NODE_SET
    ...
  END_NEW_NODE_SET
  NEW_NODE_SUBSET
    ...
  END_NEW_NODE_SUBSET
END_NODE_SET
```

2.12 Creating the node set

NEW_NODE_SET and END_NEW_NODE_SET are the key words that identify the beginning and end respectively of the data set associated with each of the sets of nodes that make up the mesh (e.g. the discretization of several bodies could be represented as a set of nodes for each body).

```
NEW_NODE_SET
  NAME = <node set label>
  BEGIN_PARAMETERS
    <node_1> <coord_1> <coord_2> <coord_3>
    <node_1> <coord_1> <coord_2> <coord_3>
    <node_1> <coord_1> <coord_2> <coord_3>
    ...
  END_PARAMETERS
END_NEW_NODE_SET
```

- NEW_NODE_SET: is the keyword that indicates the beginning of the data that characterize the set of nodes.
- END_NEW_NODE_SET: is the keyword that indicates the end of the data that characterize the set of nodes.
- NAME: is the keyword to specify the name of the set of nodes (tag) that will identify you in the set of nodes database. Must be preceded by a word that will gain the category label. Although it is an optional parameter it is recommended and situated at the beginning of the field.
- BEGIN_PARAMETERS: Keyword employee who opened the field to interpret the data that define the set of nodes: label and coordinates.
- END_PARAMETERS: Keyword closing the field that is used to interpret the data that define the set of nodes.

Rules. *This field should appear in the data file at least once. It can contain any command or data on the set of nodes and any command or data located outside shall not be interpreted as a figure corresponding to the database of sets of nodes.*

The label that identifies the set of nodes is introduced through the NAME command in this field. Its omission is not recommended, and it assigns a default value corresponding to the word NODE_SET *followed by a number.*

A node can not belong to different sets of nodes.

*Data from the set of nodes (tags and coordinates) for the discretization are introduced into single field parameters (*BEGIN_PARAMETERS *and* END_PARAMETERS*).*

Example

```
NEW_NODE_SET
  NAME = nodeset-1
  BEGIN_PARAMETERS
    1 0.000 0.000
    2 5.000 0.000
    3 10.00 0.000
    4 0.000 5.000
    5 5.000 5.000
    6 10.00 5.000
    7 0.000 10.00
    8 5.000 10.00
    9 10.00 10.00
    10 0.000 15.00
    11 5.000 15.00
    12 10.00 15.00
  END_PARAMETERS
END_NEW_NODE_SET
```

2.13 Creating the subset of nodes

NEW_NODE_SUBSET and END_NEW_NODE_SUBSET are the key words that identify the beginning and end respectively of the data set associated with a group of nodes having some common features and will be used in the program later jointly (e.g. nodes with a same contour).

```
NEW_NODE_SUBSET
  NAME = <node subset label>
  BEGIN_PARAMETERS
    <node_1>
    <node_2>
    <node_3>
    ...
  END_PARAMETERS
END_NEW_NODE_SUBSET
```

- NEW_NODE_SUBSET: is the keyword that indicates the beginning of the data that characterize the subset of nodes.
- END_NEW_NODE_SUBSET: is the keyword that indicates the end of the data that characterize the subset of nodes.
- NAME: is the keyword to specify the name of the subset of nodes (tag) that will identify you in the cluster nodes database. Must be preceded by a word that will gain the category label. Although it is an optional parameter is recommended and is situated at the beginning of the field.

- BEGIN_PARAMETERS: Keyword which opens the field to interpret the nodes (labels) that make up the group.
- END_PARAMETERS: Keyword closing the field used to interpret the nodes (labels) that make up the group.

Rules. *This field is optional in the data file and can be declared at the base of nodes (defined by BEGIN_NODE_SUBSET and END_NODE_SUBSET), but alternatively there are other fields in the data file where they can be declared. It can contain any command or data on the subset of nodes and any command or data located outside shall not be interpreted as a figure corresponding to the database of the subset of nodes.*

The label that identifies the subset of nodes is introduced through the NAME command within this field is required.

The inclusion of a node in a subset does not mean that the node should be declared in the corresponding field to the set of nodes database.

The data for the subset of nodes (labels) for the discretization are introduced into single field parameters (BEGIN_PARAMETERS and END_PARAMETERS).

Example

```
NEW_NODE_SUBSET
  NAME = node-subset-1
  BEGIN_PARAMETERS
    1
    2
    3
    4
    5
    6
  END_PARAMETERS
END_NEW_NODE_SUBSET
```

2.14 Establishment of the Basis of Elements

BEGIN_ELEMENT_SET and END_ELEMENT_SET are the key words that identify the beginning and end of all the additional data associated with the set of elements such as type of element connectivities, material, etc.

```
BEGIN_ELEMENT_SET
  DELETE = <label for the set of elements>
  NEW_ELEMENT_SET
    <body that defines all or part of the set of elements>
  END_NEW_ELEMENT_SET
END_ELEMENT_SET
```

- BEGIN_ELEMENT_SET: is the keyword that indicates the beginning of the data for the base elements.
- END_ELEMENT_SET: is the keyword that indicates the end of the data for the base elements.
- DELETE: This is the keyword to specify the name of the set of elements (tag) to be removed from the database. Must be preceded by the label for the set of elements to delete.
- NEW_ELEMENT_SET: Keyword which opens the field to the data that define a set of elements of the database (see section Creating the "Set of Elements").
- END_NEW_ELEMENT_SET: Key word here closes the field with the data that define a set of elements of the database (see section Creating the "Set of Elements").

Rules. *This field allows you to communicate with the database set containing elements data associated with elements or equivalent (e.g. mesh type, the order of integration, design, etc). This may be repeated as necessary or* DELETE *commands* NEW_ELEMENT_SET *and* END_NEW_ELEMENT_SET.

Example

```
BEGIN_ELEMENT_SET
  DELETE = element_set_1
  DELETE = element_set_2
  NEW_ELEMENT_SET
    ...
  END_NEW_ELEMENT_SET
  NEW_ELEMENT_SET
    ...
  END_NEW_ELEMENT_SET
END_ELEMENT_SET
```

2.15 Creating the set of elements

NEW_ELEMENT_SET and END_NEW_ELEMENT_SET are the key words that identify the beginning and end respectively of the data set associated with each of the sets of elements of the mesh (e.g. the discretization of several bodies are represented with a set of elements for each body).

```
NEW_ELEMENT_SET
  NAME = <element set label>
  TYPE = <type of element set>
  FORMULATION = <problem formulation>
  SUBTYPE = <subtype of element set>
  QUADRATURE = <quadrature type>
  NGAUS = <number of integration points>
  MGAUS = <number of mass matrix integr. points>
  BEGIN_PARAMETERS
    <node_1> <node_2> ... .. <node_n> <section>
    <node_1> <node_2> ... .. <node_n> <section>
    <node_1> <node_2> ... .. <node_n> <section>
    ...
  END_PARAMETERS
END_NEW_ELEMENT_SET
```

- NEW_ELEMENT_SET: is the keyword that indicates the beginning of the data that characterize the set of elements.
- END_NEW_ELEMENT_SET: is the keyword that indicates the end of the data that characterize the set of elements.
- NAME: is the keyword to specify the name of the set of elements (tag) that will identify the set in the database set of elements. Must be preceded by a word that will gain the category label. It is a mandatory parameter and is recommended to be located at the beginning of the field.
- TYPE: is the keyword to specify the type of elements of the set, and therefore that data that is needed and should be interpreted. Must be preceded by a keyword predefined by the program depending on the set of elements. It is a mandatory parameter and is recommended to be located at the beginning of the field with the only restriction to be declared before the BEGIN_PARAMETERS field and other parameters for the type of elements. The elements that are currently available are:
  - E2DSTD: 2D standard isoparametric element.

  - E2DPFEM: 2D isoparametric particle element (PFEM).
  - E3DSTD: 3D standard isoparametric element.
  - E3DPFEM: 3D isoparametric particle element (PFEM).

- FORMULATION: This is the keyword that indicates the type of formulation used for the set of elements in question and must be preceded by a keyword predefined by the program according to the formulation. Currently, the program takes into account the following:

  - SMALL_STRA_SMALL_DISP_LA: Formulation for an updated Lagrangian with small deformations and small displacements.
  - SMALL_STRA_SMALL_DISP_LT: Formulation for a total Lagrangian with small deformations and small displacements.
  - LARGE_STRA_LARGE_DISP_LA: Formulation for an updated Lagrangian with large deformations and large displacements.
  - SMALL_STRA_SMALL_DISP_LT_WSDA: Formulation for a total Lagrangian with small deformations and small displacements, plus the capacity to generate weak and strong discontinuities.

- SUBTYPE: the keyword to specify the type of element within the category of elements E2DSTD and must be preceded by a keyword predefined by the program according to the type of item. Currently, the program takes into consideration the following types:

  - LINEAR_TRIANGLE: 3-node triangular element.
  - LINEAR_QUAD: Element 4 square nodes.

- QUADRATURE: is the keyword to specify the quadrature type used for integration and should be preceded by a keyword predefined by the program depending on the quadrature rule. Currently, the program takes into consideration the following types:

  - GAUSS: Gauss-Legendre Quadrature

- NGAUS: is the keyword to specify the number of integration points and should be preceded by a positive integer.

- MGAUS: is the keyword to specify the number of integration points of the mass matrix and should be preceded by a positive integer.

- BEGIN_PARAMETERS: Keyword employee who opened the field to interpret the data that define the set of elements such as grid connectivity.

- END_PARAMETERS: Keyword closing the field used to interpret the data that define the set of elements.

Rules. *This field can contain any command or data on the set of elements and any command or data located outside shall not be interpreted in relation to a database of sets of elements.*

It is mandatory to define a label that identifies the set of elements, which is achieved through the NAME *command in this field. Failure generates an error in input reading that will stop the program.*

It is also mandatory to define the type of elements set by the TYPE *command, the omission of which also generates a read error that stops the execution.*

*Depending on the type of element, some additional commands to be used to define the set of elements. Furthermore, data from the set of elements for the discretization are introduced into a single field parameters (*BEGIN_PARAMETERS *and* END_PARAMETERS*).*

The FORMULATION SMALL_STRA_SMALL_DISP_LT_WSDA *is only implemented for the element type* E2DSTD*.*

Example

```
NEW_ELEMENT_SET
  NAME = set_elements_1
  TYPE = E2DSTD
  FORMULATION = Small_Stra_Small_Disp_LA
  SUBTYPE = Linear_Triangle
  BEGIN_PARAMETERS
    1 2 4 Section_1
    2 5 4 Section_1
    2 3 5 Section_1
    3 6 5 Section_2
    4 5 7 Section_1
    5 8 7 Section_1
    5 6 8 SECTION_2
    6 9 8 SECTION_2
    7 8 10 Section_2
    8 11 10 Section_2
    8 9 11 Section_2
    9 12 11 Section_2
  END_PARAMETERS
END_NEW_ELEMENT_SET
```

2.16 Creating the boundary conditions

BEGIN_BOUNDARY_CONDITIONS and END_BOUNDARY_CONDITIONS are the key words that identify the beginning and end respectively of the data set associated with the boundary conditions.

```
BEGIN_BOUNDARY_CONDITIONS
  BEGIN_DOF_CONDITIONS
    <Def. degrees of freedom imposed (Dirichlet conditions)>
  END_DOF_CONDITIONS
  BEGIN_ADD_NODE_SUBSET
    DELETE_SUBSET = <label of subset to eliminate>
    NEW_NODE_SUBSET
      <body of nodes set with imposed DOF>
    END_NEW_NODE_SUBSET
  END_ADD_NODE_SUBSET
END_BOUNDARY_CONDITIONS
```

- BEGIN_BOUNDARY_CONDITIONS: is the keyword that indicates the beginning of the data corresponding to the definition of boundary conditions.
- END_BOUNDARY_CONDITIONS: is the keyword that indicates the end of the data corresponding to the definition of boundary conditions.
- BEGIN_DOF_CONDITIONS: is the keyword that indicates the beginning of the data corresponding to the definition of the Dirichlet conditions for specific degrees of freedom (such as a standard displacement of solids).
- END_DOF_CONDITIONS: is the keyword that indicates the end of the data corresponding to the definition of the Dirichlet conditions for specific degrees of freedom.
- BEGIN_ADD_NODE_SUBSET: is the keyword that indicates the beginning of the data to manage the subset of nodes of the corresponding node database.
- END_ADD_NODE_SUBSET: is the keyword that indicates the end of data to manage the subset of nodes of the corresponding node database.

- DELETE_SUBSET: is the keyword to specify the name of the subset of nodes (label) to be removed from the database. Must be preceded by the label for the subset of nodes to remove. This parameter must be contained in the BEGIN_ADD_NODE_SUBSET and END_ADD_NODE_SUBSET.
- NEW_NODE_SUBSET: Keyword which opens the field with the data defining a group of nodes in the database (see section Creating the "Subset of Nodes"). This field must be contained between BEGIN_ADD_NODE_SUBSET and END_ADD_NODE_SUBSET.
- END_NEW_NODE_SUBSET: Key word here closes the field with the data defining a group of nodes (see section Creating the "Subset of Nodes"). This field must be contained between BEGIN_ADD_NODE_SUBSET and END_ADD_NODE_SUBSET.

Rules. *This field allows you to communicate with the database that defines the contour, allowing you to create, modify or delete the contour of each stage. For that reason, this field may contain other fields such as DOF. (or others that are planned in the future) This field may be absent but can never be repeated.*

As a general rule, the condition defined on a contour of the degrees of freedom of a particular problem will continue in subsequent phases unless the condition is explicitly removed or modified to that degree of freedom.

Example

```
BEGIN_BOUNDARY_CONDITIONS
  BEGIN_DOF_CONDITIONS
    ...
  END_DOF_CONDITIONS
END_BOUNDARY_CONDITIONS
```

2.17 Allocation of conditions on the degrees of freedom

BEGIN_DOF_CONDITIONS and END_DOF_CONDITIONS are the key words that identify the beginning and end of all the data associated with the contour on the degrees of freedom.

```
BEGIN_DOF_CONDITIONS
  DELETE: CURVE = <label of curve to eliminate>
  NEW_CURVE
    <bodyefining new curve>
  END_NEW_CURVE
  DELETE: NODE = <node> DOF1 DOF2 ... DOFn
  DELETE: NODE_SUBSET = <label> DOF1 DOF2 ... DOFn
  DELETE: RESET_ALL_DOF
  CREATE: NODE = <node> /
          DOF1 = [REAL <value>] [WORD: <curve label>] /
          FACTOR_DOF1 <value> = /
          DOF2 = [REAL <value>] [WORD: <curve label>] /
          FACTOR_DOF2 = <value>
  CREATE: NODE_SUBSET = <label of node subset> /
          DOF1 = [REAL <value>] [WORD: <curve label>] /
          FACTOR_DOF1 = <value> /
          DOF2 = [REAL <value>] [WORD: <curve label>] /
          FACTOR_DOF2 = <value>
END_DOF_CONDITIONS
```

- BEGIN_DOF_CONDITIONS: is the keyword that indicates the beginning of the data corresponding to the definition of the conditions imposed on the degrees of freedom.
- END_DOF_CONDITIONS: is the keyword that indicates the end of the data corresponding to the definition of the conditions imposed on the degrees of freedom.

- NEW_CURVE: Keyword that paves the way to interpret a curve (see Definition field curves).
- END_NEW_CURVE: Key word here closes the field of curves which specify the conditions on the contour of degrees of freedom.
- DELETE: This is the keyword to specify that it will eliminate a curve or a contour of the database. This option must be accompanied by one of the following keywords:
  - CURVE: Keyword to specify removal of a curve. This word should be followed by the label of the curve you want to delete.
  - RESET_ALL_DOF: Keyword to specify removal of all conditions imposed on the degrees of freedom defined in steps (stages) above as well as curves that are associated.
  - NODE: Keyword to specify removal of conditions imposed on a node. This keyword must be followed by the number of the node followed by the word / s key that identifies the degree of freedom to be eliminated. You can delete all or some of the contour of the node.
  - NODE_SUBSET: Keyword to specify removal of conditions imposed on all the nodes that comprise the subset of nodes specified. This keyword should be followed by the label that identifies the grouping of nodes (subset), followed by the word key that identifies the degree of freedom to be eliminated. As was the case above, it can remove some or all the contour of the subset.
- CREATE: is the keyword to specify that you will create a contour. This option must be accompanied by one of the following keywords:
  - NODE: Keyword to specify the node on which it is required to define the boundary conditions. This keyword must be followed by the number of the node followed by the word / key that identifies the degree of freedom to be prescribed, after the KEY is specified the size of the prescription that can be defined through a numerical value or through a curve. In the case of a numeric value, type the keyword followed by the REAL value, whereas if it is a curve, type the keyword followed by the label WORD of the curve. Moreover, it can be possible (not mandatory) to specify a factor that modifies the value. To do this, use the keyword composed of the root FACTOR and the keyword that specifies the degree of freedom, followed by the numeric value of the defined factor.

    Also on this node and on the same line of data file one or more of the contour can be created, each of which corresponds to the degree of freedom to be restricted.
  - NODE_SUBSET: Keyword to specify the subset of nodes on which one needs to define the boundary conditions. This keyword should be followed by the label that identifies the grouping of nodes (subset), followed by the word / key that identifies the degree of freedom to be prescribed, after the KEY is specified the prescription that can be defined through a numerical value or through a curve. In the case of a numeric value, type the keyword followed by the REAL value, whereas if it is a curve, type the keyword followed by the label WORD of the curve. In addition, you can specify a factor (not required) amending the prescribed value. To do this, use the keyword composed of the root FACTOR and the keyword that specifies the degree of freedom, followed by the numeric value that defines the factor.

    As was the case earlier on this group of nodes (subset) and on the same line of data file one or more conditions can be created on the contour subset of nodes, each of which corresponds to the degree of freedom to be restricted.
- Currently, the program considers the following keywords to identify the degrees of freedom:
  - DISP_X: Displacement in the X direction or first coordinate axis.
  - DISP_Y: Displacement in the Y direction or second coordinate axis.

– DISP_Z: Displacement in the Z direction or third coordinate axis.

Rules. *This field allows you to communicate with the database that defines the conditions imposed on the contour of degrees of freedom of the problem, allowing you to create, modify or delete these conditions. In this connection it must be borne in mind that if not erased, they remain in memory during the following stages. Moreover, if the data of previous stages is already stored in a memory, once it reads back the data file, the information it had in memory is overwritten.*

This field contains an independent basis curves that is managed with the commands DELETE: to remove curves and NEW_CURVE, END_NEW_CURVE to create curves and you can define as many times as needed. However, this base curve is only accessible through the field BEGIN_DOF_CONDITIONS and END_DOF_CONDITIONS.

Example

```
BEGIN_DOF_CONDITIONS
  NEW_CURVE
    NAME = disp
    TYPE = BYPOINTS
    BEGIN_PARAMETERS
      0.00 0.00
      1.00 0.25
      2.00 1.00
    END_PARAMETERS
  END_NEW_CURVE
  CREATE: NODE = 2 DISP_X = REAL: 0.0 DISP_Y = REAL: 0.0
  CREATE: NODE = 7 DISP_X = REAL: 0.0
  DELETE: NODE = 1 DISP_Y
  DELETE: NODE = 15 DISP_X DISP_Y
  DELETE: NODE = 16 DISP_Y
  CREATE: NODE = 3 = DISP_X WORD: disp DISP_Y = REAL: 1.0 /
          FACTOR_DISP_X = 2.0
  CREATE: NODE = 9 = DISP_X WORD: disp
END_DOF_CONDITIONS
```

2.18 Creating the localization data module

BEGIN_LOCALIZATIONDATA and END_LOCALIZATIONDATA identify, respectively, the beginning and the end of the strain injection parameters.

```
BEGIN_LOCALIZATIONDATA
  DIS_INJ_TYPE = <injection type>
  TAU_MXD = <tau for regular zone>
  TAU_LOC = <tau for localization>
  Q_INJECTION = <q for injection>
  Q_INF = <q at infinity>
  NORMAL_REFERENCE  NX= <x component>  NY= <y component>
  PARAK = <bandwidth fraction>
END_LOCALIZATIONDATA
```

- BEGIN_LOCALIZATIONDATA: is the keyword to specify the beginning of the field of strain injection data.
- END_LOCALIZATIONDATA: is the keyword to specify the end of the field of strain injection data.
- DIS_INJ_TYPE: is the command to indicate the strain injection type. Currently, the code has the following options:
  - WD_inj

  - SD_inj
  - Sym_SD_inj
  - No_dis_inj

- TAU_LOC: is the command to indicate the value of τ_{loc} for the first injection.
- TAU_MXD: is the command to indicate the value of τ_{mxd} for the elements that has not been injected.
- Q_INJECTION: is the command to specify the value of q_{inj}, which indicate the moment for injection.
- Q_INF: is the command to specify the lowest value of q.
- NORMAL_REFERENCE: is the command to specify the Cartesian components of the vector of reference that will help to choose the direction of discontinuity $\boldsymbol{n}$. NX refers to component x, and NY to the component y of the vector.
- PARAK: is the command to specify the band width in Strong Discontinuities Analysis, as a fraction of $l^{(e)}$.

Rules. *All parameters TAU_MXD, TAU_LOC, Q_INJECTION, Q_INF, and PARAK must have values between 0.0 and 1.0.*

Example

```
BEGIN_LOCALIZATIONDATA
  DIS_INJ_TYPE = SD_inj
  TAU_MXD = 0.1
  TAU_LOC = 0.0
  Q_INJECTION  = 0.70
  Q_INF = 0.1
  NORMAL_REFERENCE  NX= 0.70710678  NY= -0.70710678
  PARAK = 1.00
END_LOCALIZATIONDATA
```

Chapter 3

`commatfail` problemtype for GiD

The `commatfail` problemtype is an user-interface specifically designed for the pre-processor GiD. Using this interface is possible to prepare the data-file for the mechanical solver `commatfail`. The result files obtained from the analysis can be loaded in the post-processing window of GID. Using this interface it is possible to run a mechanical analysis according to the following steps:

- Geometry definition: it is possible to create and/or import the CAD geometry that defines the mechanical system to be analyzed.
- Materials: it is possible to select from a material data-base the material properties to be assigned to each volume previously defined. It is also possible to modify the material properties according to the user specification.
- Conditions: the user should assign corresponding loading and boundary conditions.
- Finite element mesh: a finite element mesh can be generated for both 2D and 3D analysis.

3.1 Problemtype instalation

Before trying to do anything, the user need to have the pre and post processor GiD installed in the computer. It can be freely downloaded from `http://www.gidhome.com`.

All the configuration files of the problemtype are in the folder `commatfail.gid`. The only thing the user have to do to install the `commatfail` problemtype is place that folder into the corresponding problemtypes folder of GiD:

Windows : `c:\Program Files\<GiD_directory>\<GiD_version>\problemtypes`

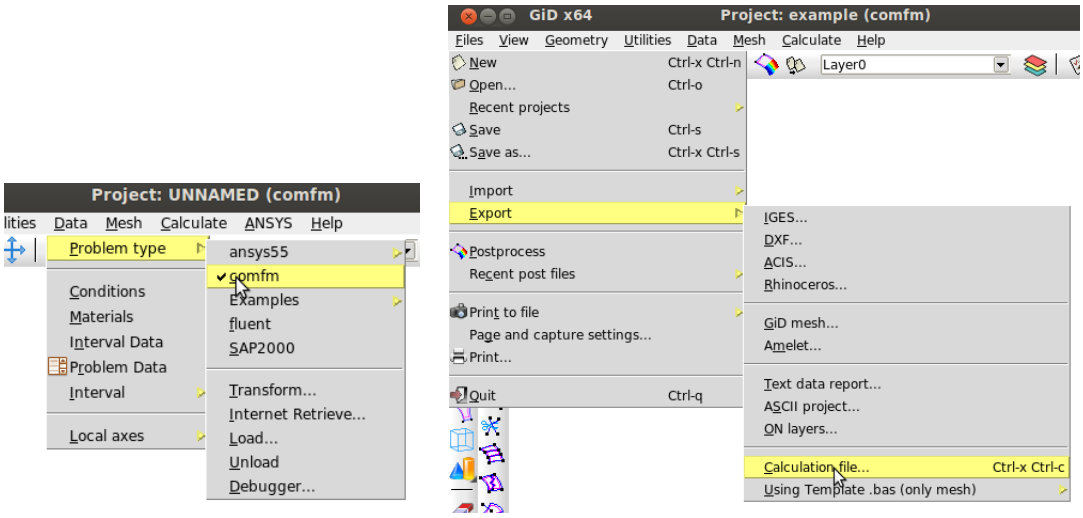
Linux : `<GiD_directory>/<GiD_version>/problemtypes`

MacOS : `Applications/<GiD_directory>/<GiD_version>/problemtypes`

Restart GiD to complete installation.

3.2 Loading the `commatfail` problemtype

To load `commatfail` problemtype interface, choose from the top menu: ***Data*** > ***Problem type*** > ***commatfail***. When pre-process is finished, the user can generate the `commatfail` input file by choosing from the top menu: ***Files*** > ***Export*** > ***Calculation Files...***, and save the `*.dat` input file.



(a) load problemtype **(b)** export file

Figure 3.1: Loading the problemtype and exporting the `*.dat` input file

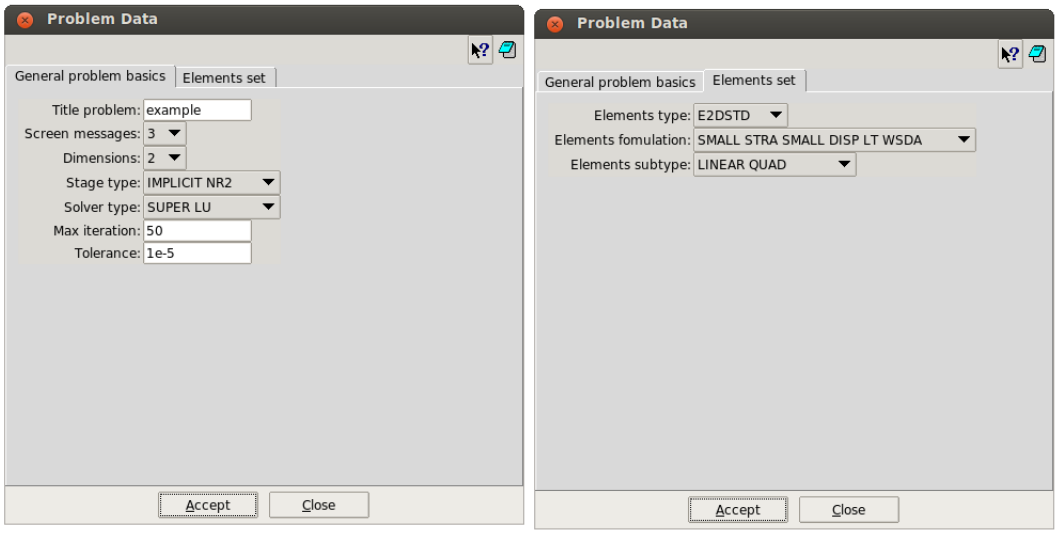
Within this pre-processor it is either possible to import a CAD geometry (IGES, DXF, etc.) or design a new one with all the CAD tools usually available in any CAD system.

3.3 Using the `commatfail` problemtype

Once the user have loaded the problemtype, he will have the options that `commatfail` will need to perform the calculations. Next, the problemtype interface is described.

3.3.1 Problem Data window

Access it with the top menu: ***Data*** > ***Problem Data***



(a) General problem basics **(b)** Elements set

Figure 3.2: Problem data window for `commatfail` problemtype

This window deals with the definition of the analysis to be performed. *General problem basics*, and *Elements set cards are available*:

General problem basics

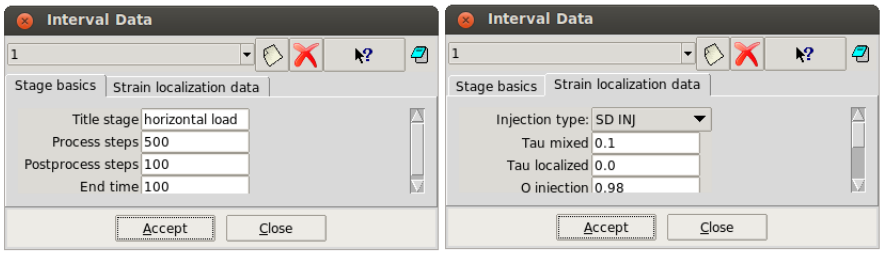
- Title problem: Field to specify some name or title to the problem. It can contain spaces, and it is recommended to use only alphanumeric characters.
- Screen messages: This option allows the user to choose the quantity of messages to be shown on the screen while the calculus is running.
- Dimensions: Use this option to specify the geometrical dimension of the problem: 1D, 2D, 3D.
- Stage type: Use this option to specify the type of calculation to be used in the analysis.
- Solver type: Use this option to specify the type of solver that the user want to use in the analysis when solving the finite element matrix equations.
- Max iteration: Specify in this field the maximum number of iterations allowed in each time-step.
- Tolerance: Specify in this field the accuracy that define a tolerance (precision) for the non-linear solver.

Elements set

- Elements type: Choose the type of elements of the problem. The type of element should be consistent with the dimension of the test.
- Elements formulation: Choose the finite element formulation to be executed for the problem.
- Elements subtype: Chose the subtype of elements if any.

3.3.2 Interval Data window

Access it with the top menu: ***Data*** > ***Interval Data***



(a) Stage basics **(b)** Strain localization data

Figure 3.3: Interval data window for commatfail problemtype

This window deals with the definition of the general data of each stage of load to be performed. Outside the window, some actions over stages are:

- ***Data*** > ***Interval*** > ***New***: creates a new load stage.
- ***Data*** > ***Interval*** > ***Current***: defines which load stage is the actual one.
- ***Data*** > ***Interval*** > ***Delete***: deletes a load stage.

Stage basics, and *Strain localization data* cards are available:

Stage basics

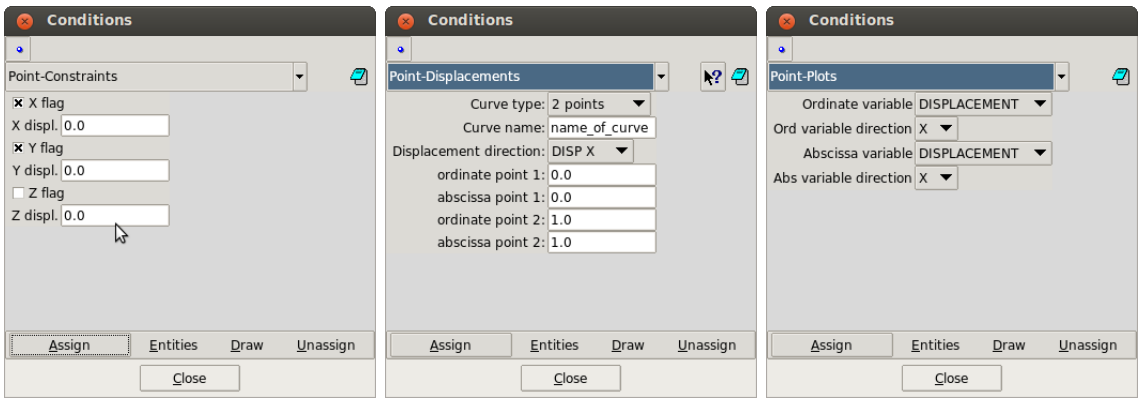
- Title stage: Write in this field a title to the stage. It serve the user to remember what happens in that stage or to distinguish it from the others. This field can contain spaces, and it is strongly recommended to use only alpha-numeric characters.
- Process steps: Specify here the number of steps of the stage. Increasing this number will increase both the time of the analysis and the quality of the results.
- Post-process steps: Specify here how many of the process steps will be in the post-process. It must never be higher than the process steps.
- End time: Specify the final time for the stage so the analysis can compute the size of each time-step in the actual stage.

Strain localization data

- Injection type: Choose here the type of injection for the material failure process.
- Tau mixed: White the value of the stabilization parameter for the regular zone. The moment of the first strain injection (bifurcation time).
- Tau localized: White the value of the stabilization parameter for the localized zone. The second injection (strain discontinuity).
- Q injection: Specify the fraction of q to inject the reduced integration.
- Q infinite: Specify the fraction of q to inject the strong discontinuity.
- Normal reference: Specify the two Cartesian components for the reference normal vector.
- Parameter K: Write the fraction of the element size for strong discontinuity band width.

3.3.3 Conditions window

Access it with the top menu: ***Data*** > ***Conditions***



(a) Constraints **(b)** Displacements **(c)** Plots

Figure 3.4: Conditions window for `commatfail` problemtype

Opening the condition window the user will be able to assign constraints, plots or imposed displacements to points of the mesh.

Point constraints

The Point-Constraints condition should be used to assign the boundary conditions to the geometry.

Point plots

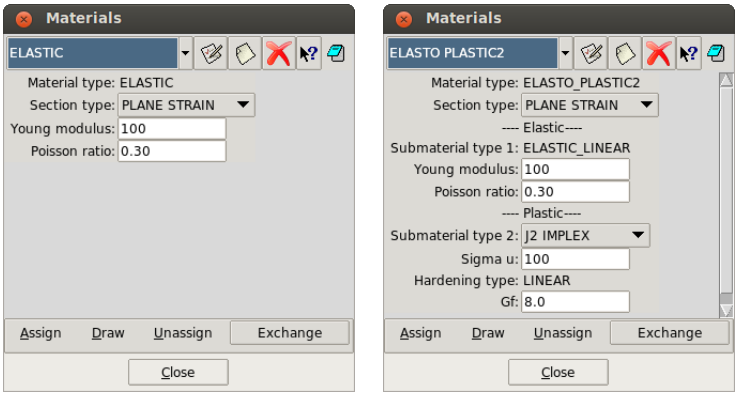
The Point-Plots condition can be used to specify any curve the user wants to plot after the analysis.

Point displacements

The Point-Displacements condition should be used to impose some known displacement to any point in the mesh. The displacement can be defined by a 2, 3, 4, or 5 points curve.

3.3.4 Materials window

Access it with the top menu: ***Data*** > ***Materials***



(a) Elastic **(b)** Elastop-plastic

Figure 3.5: Materials window for `commatfail` problemtype

Chapter 4

User example for `commatfail`

4.1 Problem to solve

Here we will sole step by step the problem sketched on the Figure 4.1.

Figure 4.1: Sketch of the problem to solve

4.2 Generating the input file

The following steps will guide the user through the geometry generation and the assignment of the required properties for this example. All these steps should be done in GiD, after the installation of `commatfail` problemtype.

1. Create a new file: ***File*** > ***New***

2. Create the geometry:

   (a) ***Geometry*** > ***Create*** > ***Object*** > ***Rectangle***

   (b) To create the first corner of the rectangle, write into the command line: `0,0 + enter`

   (c) To create the second corner of the rectangle, write into the command line: `4,2 + enter`

   The screen should look like the one shown in Figure 4.2.

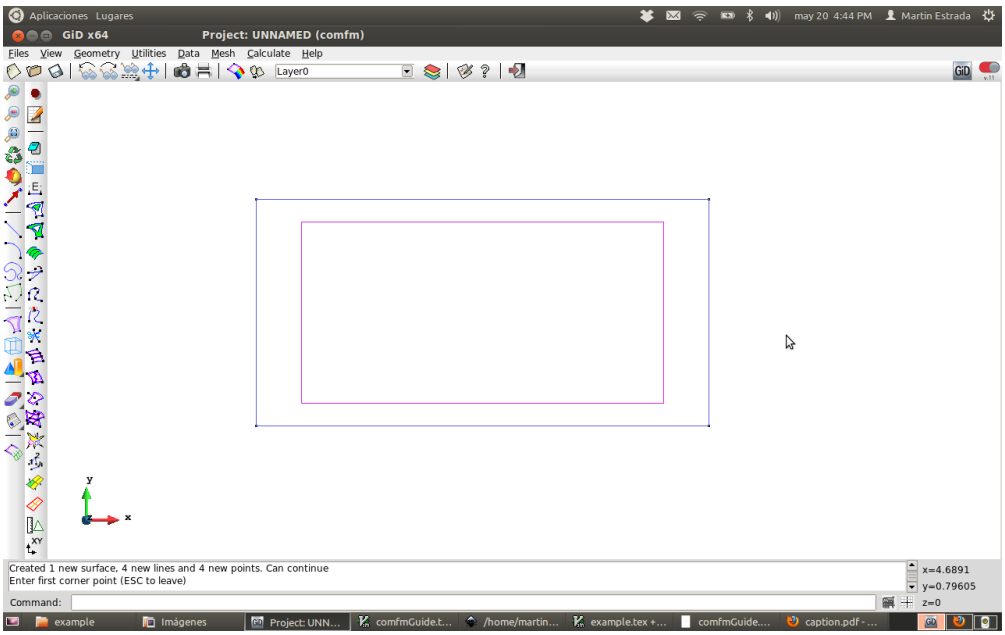
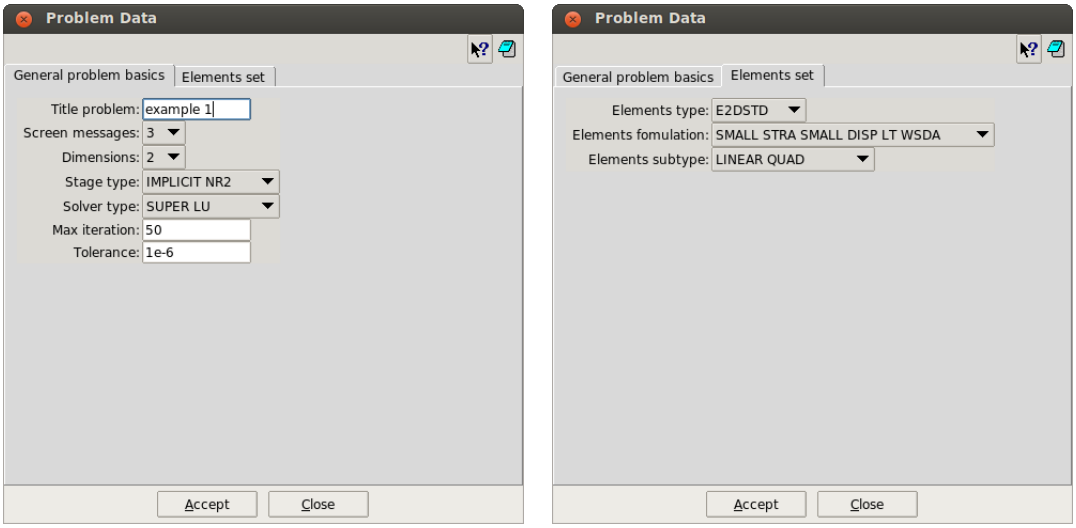


Figure 4.2: Geometry of the problem

3. Load the `commatfail` problemtype: ***Data*** > ***Problem type*** > ***commatfail***

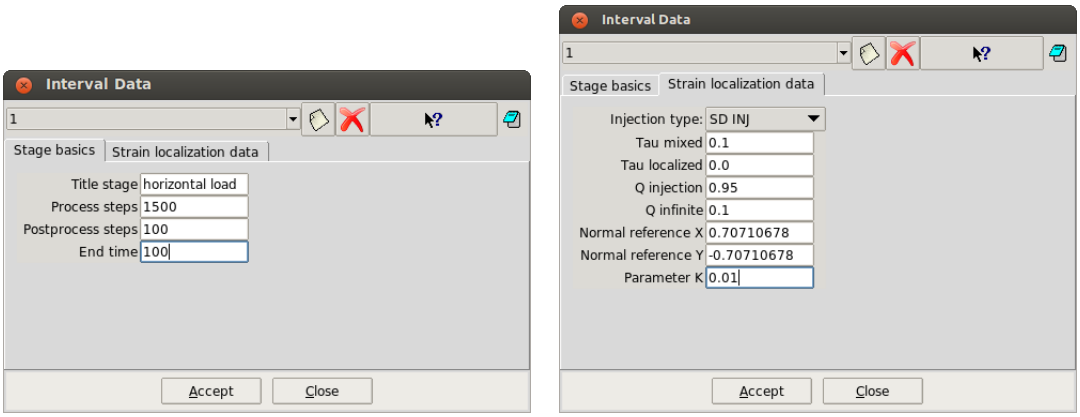
4. Establish the problem data: ***Data*** > ***Problem data***



(a) General problem basics **(b)** Elements set

Figure 4.3: Problem data

5. Establish the interval data: ***Data*** > ***Interval data***



(a) Stage basics **(b)** Strain localization data

Figure 4.4: Interval data

6. Create the mesh: Use the GiD tools from the top menu ***Mesh*** to create a structured mesh that look like the one on Figure 4.5.

   (a) Establish a structured mesh: ***Mesh*** > ***Structured*** > ***Surfaces*** > ***Assign number of cells***

   (b) Select the created rectangle surface + esc

   (c) Enter the number 4 + Assign

   (d) Select the vertical left line + esc

   (e) Enter the number 8 + Assign

   (f) Select the horizontal top line + esc

   (g) Generate the mesh: ***Mesh*** > ***Generate mesh***

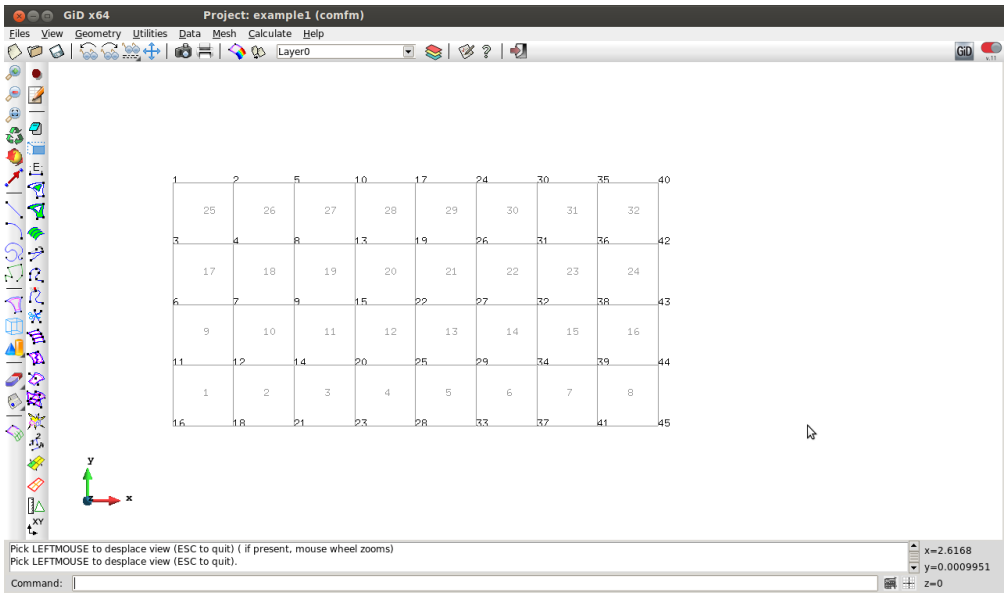

GiD x64
Project: example1 (comfm)
Files View Geometry Utilities Data Mesh Calculate Help
Layer0
Pick LEFTMOUSE to desplace view (ESC to quit) (if present, mouse wheel zooms)
Pick LEFTMOUSE to desplace view (ESC to quit).
Command:
x=2.6168
y=0.0009951
z=0

Figure 4.5: Mesh of the problem

7. Assign the point constraints to some points: ***Data*** > ***conditions*** + Point-Constraints condition:

   (a) $x = 0.0$ and $y = 0.0$

(b) Assign + Select the 5 left points (1, 3, 6, 11, 16) + Finish

8. Assign known displacement to some points: ***Data*** > ***conditions*** + Point-Displacement condition:

   (a) Specify the properties of the displacement curve

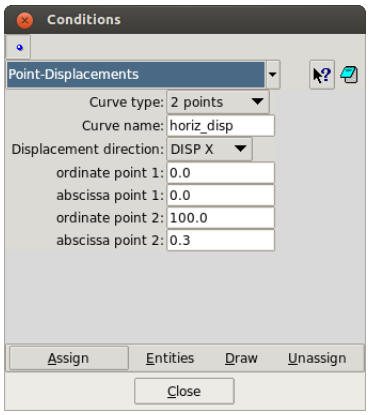


Figure 4.6: Displacement curve properties

   (b) Assign + Select the 5 right points (40, 42, 43, 44, 45) + Finish

9. Assign a point to create a force-displacement plot: ***Data*** > ***conditions*** + Point-Plots condition:

   (a) Specify the properties of the plot

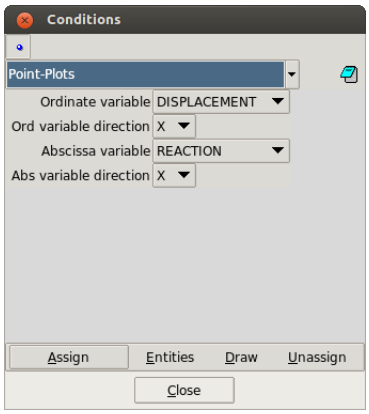
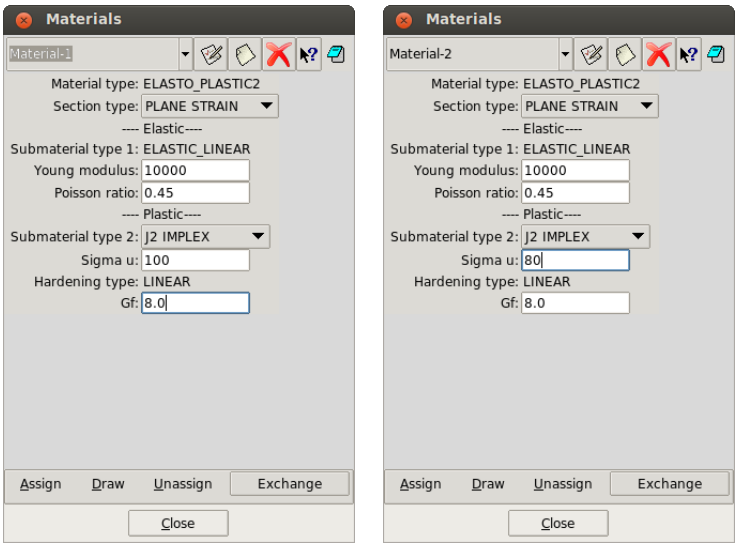


Figure 4.7: Plot properties

   (b) Assign + Select the point 43 + Finish

10. Materials: ***Data*** > ***Materials***

    (a) Create two new materials of type elasto-plastic with the properties on Figure 4.8



(a) Material 1 **(b)** Material 2

Figure 4.8: Creation of two new material of elasto-plastic type

(b) Assign Material 2 to element number 4

(c) Assign Material 1 to all other elements

11. Generate input file: ***Files*** > ***Export*** > ***Calculation file...***

4.3 Input file

The input file to run this example was generated with `commatfail` probemtype, and is shown below. It can also be found as `example1.dat` in the folder `examples` that comes with the download.

```
! ======================================================================
!
! File generated by commatfail.gid problemtype
!
! Input file for problem: example 1
!
! ======================================================================

BEGIN_PROBLEM


  ! Basic problem information
  ! -------------------------
  BEGIN_PROBLEM_BASICS
    TITLE = example 1
    SCRLEVEL = 3 ! screen messages level
    RSNLEVEL = 3 ! rsn file messages level
    NDIME = 2 ! problem dimension
    STAGE_TYPE = IMPLICIT_NR2 ! stage type (existing types --> stgtype)
    SOLVER_TYPE = SUPER_LU ! solver type (existing types --> solvtype)
    MAX_ITERATION = 50 ! maximum iterations for convergence
    TOLERANCE = 1e-6 ! tolerance level for convergence
  END_PROBLEM_BASICS


  ! ------------------------------------------------------------------
  ! Stage: horizontal load
  ! ------------------------------------------------------------------
  NEW_STAGE
```

```
! Stage basic information
! ------------------------
BEGIN_STAGE_BASICS
  TITLE = horizontal load
  NUMBER_STEPS = 600 ! time-steps (increments)
  NUMBER_POST = 100 ! postprocess time-steps
  END_TIME = 100 ! stage final time
END_STAGE_BASICS


! Materials definition
! --------------------
BEGIN_MATERIAL

  ! New material
  NEW_MATERIAL
    NAME = Mat_1 ! material label
    TYPE = ELASTO_PLASTIC2 ! material type (existing types --> mat%mtype)
    NEW_SUBMATERIAL
      NAME = Submat_el_1 ! submaterial label
      TYPE = ELASTIC_LINEAR ! submaterial type (existing types --> sbmat%stype)
      BEGIN_PARAMETERS
        YOUNG = 10000 ! young modulus
        POISSON = 0.45 ! poisson ratio
      END_PARAMETERS
    END_NEW_SUBMATERIAL
    NEW_SUBMATERIAL
      NAME = Submat_pl_1 ! submaterial label
      TYPE = J2_IMPLEX ! submaterial type (existing types --> sbmat%stype)
      BEGIN_PARAMETERS
        SIGMAU = 100.0 ! elastic limit
        HARD_TYPE = LINEAR ! hardening type
        GFVAL = 8.0 ! plastic modulus
      END_PARAMETERS
    END_NEW_SUBMATERIAL
  END_NEW_MATERIAL

  ! New material
  NEW_MATERIAL
    NAME = Mat_2 ! material label
    TYPE = ELASTO_PLASTIC2 ! material type (existing types --> mat%mtype)
    NEW_SUBMATERIAL
      NAME = Submat_el_2 ! submaterial label
      TYPE = ELASTIC_LINEAR ! submaterial type (existing types --> sbmat%stype)
      BEGIN_PARAMETERS
        YOUNG = 10000 ! young modulus
        POISSON = 0.45 ! poisson ratio
      END_PARAMETERS
    END_NEW_SUBMATERIAL
    NEW_SUBMATERIAL
      NAME = Submat_pl_2 ! submaterial label
      TYPE = J2_IMPLEX ! submaterial type (existing types --> sbmat%stype)
      BEGIN_PARAMETERS
        SIGMAU = 80.0 ! elastic limit
        HARD_TYPE = LINEAR ! hardening type
        GFVAL = 8.0 ! plastic modulus
      END_PARAMETERS
    END_NEW_SUBMATERIAL
  END_NEW_MATERIAL

END_MATERIAL


! Sections definition
```

```
! -------------------
BEGIN_SECTION

  ! New section
  NEW_SECTION
    NAME = Sec_1 ! section label
    TYPE = PLANE_STRAIN ! section type (existing types --> sec%stype)
    BEGIN_PARAMETERS
      MATERIAL = Mat_1 ! material label associated
    END_PARAMETERS
  END_NEW_SECTION

  ! New section
  NEW_SECTION
    NAME = Sec_2 ! section label
    TYPE = PLANE_STRAIN ! section type (existing types --> sec%stype)
    BEGIN_PARAMETERS
      MATERIAL = Mat_2 ! material label associated
    END_PARAMETERS
  END_NEW_SECTION

END_SECTION


! Nodes sets definition
! ---------------------
BEGIN_NODE_SET

  ! New node set
  NEW_NODE_SET
    NAME = Nodes_coord ! node set label
    BEGIN_PARAMETERS
      1              0            1
      2           0.25            1
      3              0         0.75
      4           0.25         0.75
      5            0.5            1
      6              0          0.5
      7           0.25          0.5
      8            0.5         0.75
      9            0.5          0.5
      10           0.75            1
      11              0         0.25
      12           0.25         0.25
      13           0.75         0.75
      14            0.5         0.25
      15           0.75          0.5
      16              0            0
      17              1            1
      18           0.25            0
      19              1         0.75
      20           0.75         0.25
      21            0.5            0
      22              1          0.5
      23           0.75            0
      24           1.25            1
      25              1         0.25
      26           1.25         0.75
      27           1.25          0.5
      28              1            0
      29           1.25         0.25
      30            1.5            1
      31            1.5         0.75
      32            1.5          0.5
      33           1.25            0
      34            1.5         0.25
```

```
      35          1.75            1
      36          1.75         0.75
      37           1.5            0
      38          1.75          0.5
      39          1.75         0.25
      40             2            1
      41          1.75            0
      42             2         0.75
      43             2          0.5
      44             2         0.25
      45             2            0
    END_PARAMETERS
  END_NEW_NODE_SET

END_NODE_SET


! Elements sets definition
! ------------------------
BEGIN_ELEMENT_SET

  ! New element set
  NEW_ELEMENT_SET
    NAME = Elem_set_1 ! element set label
    TYPE = E2DSTD ! element set type (existing types --> esetyp)
    FORMULATION = SMALL_STRA_SMALL_DISP_LT_WSDA ! element set formulation (existing types --
    SUBTYPE = LINEAR_QUAD ! element set subtype (existing types --> etype)
    BEGIN_PARAMETERS
      1  18 12 11 16  Sec_1
      2  21 14 12 18  Sec_1
      3  23 20 14 21  Sec_1
      4  28 25 20 23  Sec_2
      5  33 29 25 28  Sec_1
      6  37 34 29 33  Sec_1
      7  41 39 34 37  Sec_1
      8  45 44 39 41  Sec_1
      9  12 7 6 11  Sec_1
      10  14 9 7 12  Sec_1
      11  20 15 9 14  Sec_1
      12  25 22 15 20  Sec_1
      13  29 27 22 25  Sec_1
      14  34 32 27 29  Sec_1
      15  39 38 32 34  Sec_1
      16  44 43 38 39  Sec_1
      17  7 4 3 6  Sec_1
      18  9 8 4 7  Sec_1
      19  15 13 8 9  Sec_1
      20  22 19 13 15  Sec_1
      21  27 26 19 22  Sec_1
      22  32 31 26 27  Sec_1
      23  38 36 31 32  Sec_1
      24  43 42 36 38  Sec_1
      25  4 2 1 3  Sec_1
      26  8 5 2 4  Sec_1
      27  13 10 5 8  Sec_1
      28  19 17 10 13  Sec_1
      29  26 24 17 19  Sec_1
      30  31 30 24 26  Sec_1
      31  36 35 30 31  Sec_1
      32  42 40 35 36  Sec_1
    END_PARAMETERS
  END_NEW_ELEMENT_SET

END_ELEMENT_SET
```

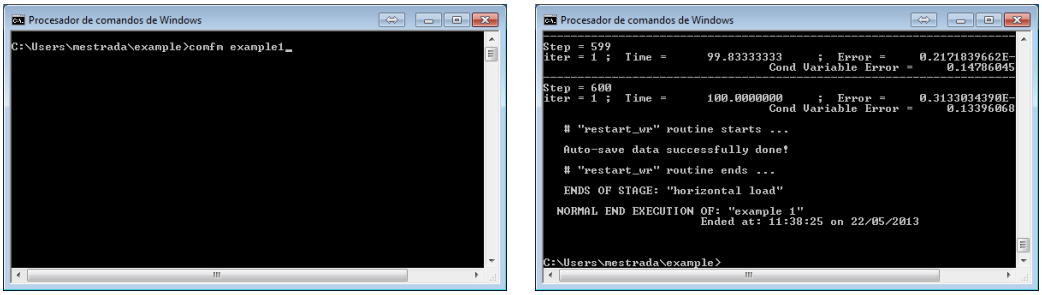
```
    ! Boundary conditions
    ! -------------------
    BEGIN_BOUNDARY_CONDITIONS

      BEGIN_DOF_CONDITIONS

        ! Constraints
        CREATE NODE = 1  DISP_X = REAL : 0.0  DISP_Y = REAL : 0.0
        CREATE NODE = 3  DISP_X = REAL : 0.0  DISP_Y = REAL : 0.0
        CREATE NODE = 6  DISP_X = REAL : 0.0  DISP_Y = REAL : 0.0
        CREATE NODE = 11  DISP_X = REAL : 0.0  DISP_Y = REAL : 0.0
        CREATE NODE = 16  DISP_X = REAL : 0.0  DISP_Y = REAL : 0.0

        ! New curve by points
        NEW_CURVE
          NAME = horiz_disp ! curve label
          TYPE = BYPOINTS ! curve type (existing types --> crv%ctype)
          BEGIN_PARAMETERS
            0.0 0.0
            100.0 0.3
          END_PARAMETERS
        END_NEW_CURVE

        ! Displacement by curves
        CREATE NODE = 40  DISP_X = WORD : horiz_disp  FACTOR_DISP_X = 1
        CREATE NODE = 42  DISP_X = WORD : horiz_disp  FACTOR_DISP_X = 1
        CREATE NODE = 43  DISP_X = WORD : horiz_disp  FACTOR_DISP_X = 1
        CREATE NODE = 44  DISP_X = WORD : horiz_disp  FACTOR_DISP_X = 1
        CREATE NODE = 45  DISP_X = WORD : horiz_disp  FACTOR_DISP_X = 1

      END_DOF_CONDITIONS

    END_BOUNDARY_CONDITIONS


    ! Strain localization data
    ! ------------------------
    BEGIN_LOCALIZATIONDATA

      DIS_INJ_TYPE = SD_INJ ! injection type (existing types --> dis_inj_type)
      TAU_MXD = 0.1 ! tau for regular zone (0-1)
      TAU_LOC = 0.0 ! tau for localized zone (0-1)
      Q_INJECTION = 0.95 ! fraction of q to inject reduced integration [0-1]
      Q_INF = 0.1 ! fraction of q to inject strong discontinuity [0-1]
      NORMAL_REFERENCE NX = 0.70710678 NY = -0.70710678 ! reference normal vector
      PARAK = 0.01 ! fraction of element size for strong discontinuity band width (0-1)

    END_LOCALIZATIONDATA


    ! Plots definition
    ! ----------------
    BEGIN_PLOTS

      ! New plot
      NEW_PLOT
        X-AXIS DISPLACEMENT : NODE = 43 F_X
        Y-AXIS REACTION : NODE = 43 F_X

      END_PLOT

    END_PLOTS

  END_NEW_STAGE

END_PROBLEM
```

```
! End of file
```

4.4 Processing the problem

After having the input file, the user should have the following files in the same folder in order to make the computations: `example1.dat`, `commatfail.exe`, `commatfailpost`.

The processing phase is launched with the following command in a command prompt:
`commatfail example1` + enter
The beginning and ending of this process should look like shown in Figure 4.9

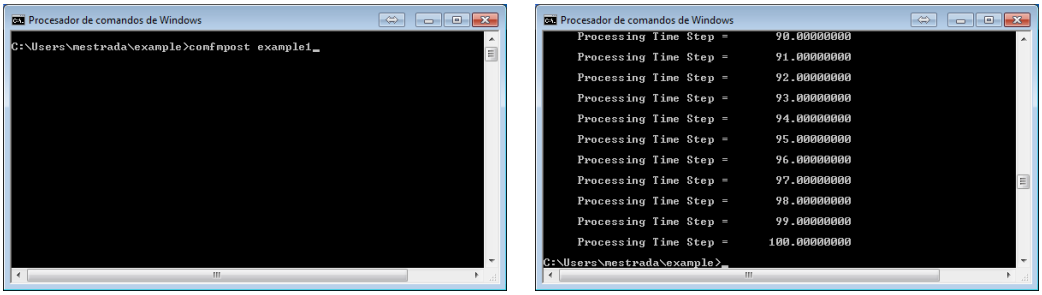

Procesador de comandos de Windows
C:\Users\mestrada\example>comfm example1_
Procesador de comandos de Windows
Step = 599
iter = 1 ; Time = 99.83333333 ; Error = 0.2171839662E-
Cond Variable Error = 0.14706045
Step = 600
iter = 1 ; Time = 100.0000000 ; Error = 0.3133034390E-
Cond Variable Error = 0.13396068
"restart_wr" routine starts ...
Auto-save data successfully done!
"restart_wr" routine ends ...
ENDS OF STAGE: "horizontal load"
NORMAL END EXECUTION OF: "example 1"
Ended at: 11:38:25 on 22/05/2013
C:\Users\mestrada\example>

(a) Begin of process **(b)** End of process

Figure 4.9: Processing the problem

4.5 Post-processing the problem

The post-processing phase is launched with the following command in the same command prompt:
`commatfailpost example1` + enter
The beginning and ending of this process should look like shown in Figure 4.10


Procesador de comandos de Windows
C:\Users\mestrada\example>comfmpost example1_
Procesador de comandos de Windows
Processing Time Step = 90.00000000
Processing Time Step = 91.00000000
Processing Time Step = 92.00000000
Processing Time Step = 93.00000000
Processing Time Step = 94.00000000
Processing Time Step = 95.00000000
Processing Time Step = 96.00000000
Processing Time Step = 97.00000000
Processing Time Step = 98.00000000
Processing Time Step = 99.00000000
Processing Time Step = 100.00000000
C:\Users\mestrada\example>

(a) Begin of process **(b)** End of process

Figure 4.10: Processing the problem

4.6 Showing the results

The additional files created during the process and post-process phases contain the information to show the results in a more user-friendly way.

4.6.1 Curve plots

Curve plot data for node 43 are stored in the files: `example1.c01`. The plot of those data is shown in Figure 4.11.

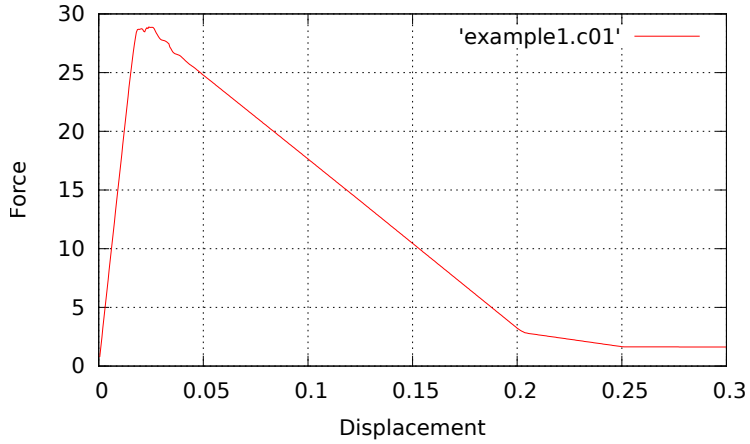
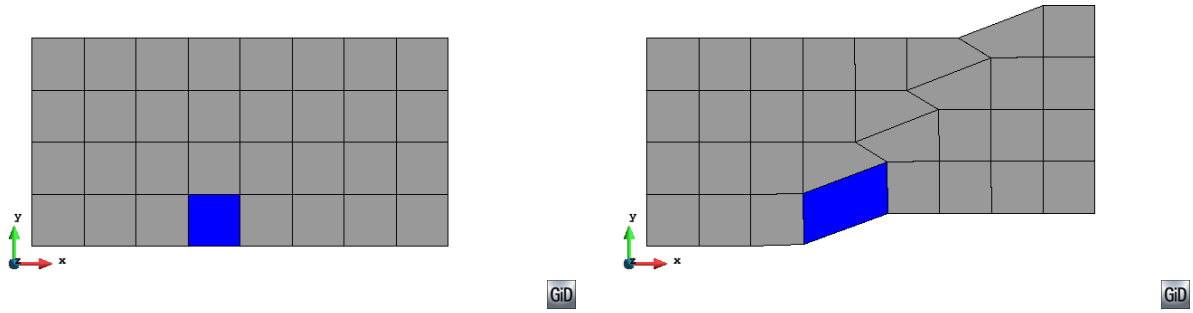


Figure 4.11: Force-Displacement curve plot for node 43

4.6.2 GiD outputs

The user have to change GiD to the post-process window in order to see the results. This can be done with the top menu ***Files*** > ***Postprocess*** or with the corresponding icon in the menu bar. Once the `*.flavia` file is loaded, GiD can show many results. Some of them are the ones in the figures below.

Deformed shape can be shown with the top menu: ***View results*** > ***Deformation*** > ***TOTAL DISP***.



(a) Undeformed shape **(b)** Deformed shape

Figure 4.12: Graphic displacement results

The crack path is shown by plotting the double smooth variable: ***View results*** > ***Contour lines*** > ***Double smoth***. Then, the minimum and maximum values should be fixed on -0.001 and 0.001, respectively.

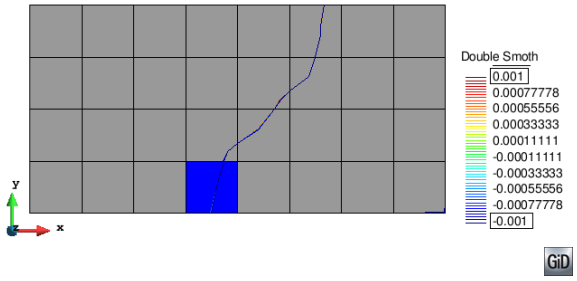
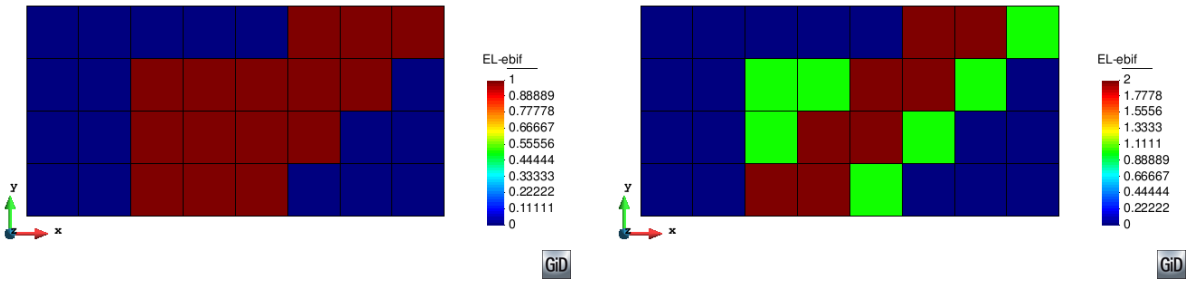


Figure 4.13: Crack path results (`Double smoth`)

The bifurcated and injected elements are shown with: ***View results*** > ***Contour fill*** > ***ebif***.



(a) Post-process step 8 **(b)** Post process step 60

Figure 4.14: Injection procedure results (`EL-ebif`)

Chapter 5

Strain injection implementation in `commatfail`

This chapter explain in a more comprehensible language than the original source `Fortran 90` files the implementation of the methods for the Strain Injection Techniques in Numerical Modeling of Propagating Material Failure. The complete formal explanation of this implementation can be found at Dias et al. (2012).

Principal subroutines related with the implementation of the strain injection techniques in `commatfail` are explained here.

5.1 Subroutine `calcimpstg_2`

5.1.1 Description

Calculate stage integration for implicit scheme.

5.1.2 Procedure

1. Initialize stage variables [`calcimpstg_init`]

   $$\boldsymbol{F}^{ext} = 0,\ \boldsymbol{F}^{int} = 0,\ \hat{\boldsymbol{R}} = 0,\ \ldots$$

2. Begin loop over time-steps (n)

   (a) Remesh if required [`remesh`]

   (b) Initialize residual variable and vector

   $$||\boldsymbol{r}|| = 0$$
   $$\hat{\boldsymbol{R}} = \mathbf{0}$$

   (c) Modify DOF by prescribed DOF in first iteration of the actual time-step (actualization of displacements) [`calc_odof`]

   $$\boldsymbol{u}_{n+1} = \boldsymbol{u}_{n+1} + \delta\boldsymbol{u}$$

   (d) Compute forces and residual vectors for initial displacement [`calc_resid_2`]

$$\boldsymbol{F}^{ext} = \underset{e\in\Omega}{\mathcal{A}}\left(\int_{\Omega^{(e)}} \boldsymbol{N}^T\,\boldsymbol{b}_{n+1}\,d\Omega + \int_{\Gamma_\sigma^{(e)}} \boldsymbol{N}^T\,\boldsymbol{t}^*_{n+1}\,d\Gamma\right) \quad [\texttt{calc\_extload}]$$

$$\boldsymbol{F}^{int} = \underset{e\in\Omega}{\mathcal{A}}\left(\int_{\Omega^{(e)}} \boldsymbol{B}^{(e)T}\,\tilde{\boldsymbol{\sigma}}^{(e)}_{n+1}\,(\Delta\boldsymbol{u}_{n+1})\;d\Omega\right),\ \boldsymbol{r} = \hat{\boldsymbol{r}}(\Delta\boldsymbol{u}_{n+1}) \quad [\texttt{cfint\_e2dstd\_sssdlt\_wsda}]$$

$$\boldsymbol{R} = \boldsymbol{F}^{ext} - \boldsymbol{F}^{int} \quad [\texttt{calc\_forctoresid}]$$

(e) Begin loop over time-step iterations (k) until the error gets lower than certain tolerance or a maximum number of iterations is complete

$||\boldsymbol{r}|| = 0$

i. Calculate stiffness matrix [calc_stiff]

$$\hat{\boldsymbol{K}} = \underset{e\in\Omega}{\mathcal{A}}\left(\hat{\boldsymbol{K}}^{(e)} = \boldsymbol{K}^{(e)}_{\boldsymbol{uu}} - \boldsymbol{K}^{(e)}_{\boldsymbol{u}[\![\boldsymbol{u}]\!]}\boldsymbol{K}^{(e)-1}_{[\![\boldsymbol{u}]\!][\![\boldsymbol{u}]\!]}\boldsymbol{K}^{(e)}_{[\![\boldsymbol{u}]\!]\boldsymbol{u}}\right) \quad [\texttt{stiff\_e2dstd\_sssdlt\_wsda}]$$

ii. Calculate condensate residual [conds_resid_e2dstd_c2]

$$\hat{\boldsymbol{R}}^k = \boldsymbol{R} - \underset{e\in\Omega}{\mathcal{A}}\left(\boldsymbol{K}^{(e)}_{\boldsymbol{u}[\![\boldsymbol{u}]\!]}\boldsymbol{K}^{(e)-1}_{[\![\boldsymbol{u}]\!][\![\boldsymbol{u}]\!]}\,\boldsymbol{r}^{(e)}\right)$$

iii. Solve the general system of equations for $\delta\boldsymbol{u}$ and $[\![\boldsymbol{u}]\!]$
IF arclength solver is used

$$\delta\boldsymbol{u}^k \leftarrow \hat{\boldsymbol{K}}\,\delta\boldsymbol{u}^k = \hat{\boldsymbol{R}}^k \quad [\texttt{arclen, actualizedof}]$$

ELSE

$$\delta\boldsymbol{u}^k \leftarrow \hat{\boldsymbol{K}}\,\delta\boldsymbol{u}^k = \hat{\boldsymbol{R}}^k \quad [\texttt{solver, actualizedof}]$$

$$[\![\boldsymbol{u}]\!]_{n+1} = \boldsymbol{K}^{-1}_{[\![\boldsymbol{u}]\!][\![\boldsymbol{u}]\!]}\left(\boldsymbol{r} - \boldsymbol{k}_{[\![\boldsymbol{u}]\!]\boldsymbol{u}}\delta\boldsymbol{u}^k\right) \quad [\texttt{act\_condsvar\_e2dstd\_c2}]$$

iv. Update displacement and increment

$$\boldsymbol{u}^k_{n+1} = \boldsymbol{u}^{k-1}_{n+1} + \delta\boldsymbol{u}^k$$
$$\Delta\boldsymbol{u}_{n+1} = \boldsymbol{u}^k_{n+1} - \boldsymbol{u}_n$$

v. Compute forces and residual vectors for actual iteration [calc_resid_2]

$$\boldsymbol{F}^{ext} = \underset{e\in\Omega}{\mathcal{A}}\left(\int_{\Omega^{(e)}} \boldsymbol{N}^T\,\boldsymbol{b}_{n+1}\,d\Omega + \int_{\Gamma_\sigma^{(e)}} \boldsymbol{N}^T\,\boldsymbol{t}^*_{n+1}\,d\Gamma\right) \quad [\texttt{calc\_extload}]$$

$$\boldsymbol{F}^{int} = \underset{e\in\Omega}{\mathcal{A}}\left(\int_{\Omega^{(e)}} \boldsymbol{B}^{(e)T}\,\tilde{\boldsymbol{\sigma}}^{(e)}_{n+1}\,(\Delta\boldsymbol{u}_{n+1})\;d\Omega\right),\ \boldsymbol{r} = \hat{\boldsymbol{r}}(\Delta\boldsymbol{u}_{n+1}) \quad [\texttt{cfint\_e2dstd\_sssdlt\_wsda}]$$

$$\boldsymbol{R} = \boldsymbol{F}^{ext} - \boldsymbol{F}^{int} \quad [\texttt{calc\_forctoresid}]$$

vi. Error calculation

$$||\boldsymbol{F}^{int}|| = \sqrt{\boldsymbol{F}^{int\,T}\ \boldsymbol{F}^{int}}$$
$$||\boldsymbol{R}|| = \sqrt{\boldsymbol{R}^{T}\ \boldsymbol{R}}$$
$$\epsilon_F = \frac{1 + ||\boldsymbol{F}^{int}||}{||\boldsymbol{R}||}$$
$$\epsilon_r = \frac{||\boldsymbol{r}||}{1 + ||\boldsymbol{F}^{int}||}$$

End loop over time-step iterations if $\epsilon_F < tol$ and $\epsilon_r < tol$

(f) Write plot info [`wroutplot_e2dstd`]

(g) Actualize converged values [`actimstg_2`]

(h) Write post-process info [`wroutpost`]

(i) Write restart file [`restart_wr`]

End loop over time-steps when stage is over

3. Write output results of last step [`wroutpost`]

5.2 Subroutine `cfint_e2dstd_sssdlt_wsda`

5.2.1 Description

Computes the vector of internal forces of elements of type E2DSTD for the symmetric and non-symmetric strong discontinuity approach. The superscript (e) in equations indicate an elemental quantity.

5.2.2 Procedure

1. Begin loop over all elements

   (a) Read previously calculated values

   $l^{(e)}$, $k^{(e)}$, $\Delta\boldsymbol{u}$, $[\![\boldsymbol{u}]\!]$, $\nabla\varphi$, $\boldsymbol{n}$, ...

   (b) Assign mixed formulation values depending on the injection stage

   $\tau^{(e)} = 0.0 \qquad \forall e \in \Omega_{inj};\ \Omega_{inj} \subset \{\Omega_{mxd}, \Omega_{Dis}\}$ [`input.dat >> TAU_LOC = 0.0`]
   $\tau^{(e)} = 1.0 \qquad \forall e \in \Omega \backslash \Omega_{inj}$ general constitutive models
   $\tau^{(e)} = 0.1 \qquad \forall e \in \Omega \backslash \Omega_{inj}$ isochoric constitutive models[`input.dat >> TAU_MXD = 0.1`]

   $\xi^{(e)} = 0.0 \qquad \forall e \in \Omega \backslash \Omega_{Dis}$
   $\xi^{(e)} = 1.0 \qquad \forall e \in \Omega_{Dis}$

   (c) Compute integration variables on each of the 6 gauss-points

$$\det\left(\boldsymbol{J}\right)_{gp} \quad [\texttt{calc\_jacob}]$$
$$dV_{gp}^{(e)} = w_{gp}\ \det\left(\boldsymbol{J}_{gp}\right)$$
$$dV^{(e)} = \sum_{gp=1}^{ngp}\left(dV_{gp}^{(e)}\right)$$
$$de = \frac{dV_6^{(e)}}{l^{(e)}}$$

(d) Calculate stress for gauss-point 5 (reduced integration scheme, representative of the stress at the discontinuity)

$$\boldsymbol{B}^{(e)} = \boldsymbol{\nabla}\boldsymbol{N} \quad [\texttt{calc\_bdef\_sssdlt\_bstd}]$$
$$\Delta\boldsymbol{\varepsilon}_{\mathcal{S}}^{(e)} = \boldsymbol{B}^{(e)}\Delta\boldsymbol{u}^{(e)} - \xi^{(e)}\left(\boldsymbol{\nabla}\varphi^h\right)^{(e)}\ [\![\boldsymbol{u}]\!]^{(e)} + \xi^{(e)}\frac{1}{h^{(e)}}\boldsymbol{n}^{(e)}\ [\![\boldsymbol{u}]\!]^{(e)}$$
$$\overline{\boldsymbol{\sigma}}_{n+1}^{(e)} = \dot{\boldsymbol{\Sigma}}\left(\boldsymbol{\nabla}^s\boldsymbol{u}^{(e)} = \Delta\boldsymbol{\varepsilon}_{\mathcal{S}}^{(e)}\right) \quad [\texttt{calc\_stress}]$$

(e) Calculate stress for gauss-point 6 (elastic process is forced once a discontinuity is injected)

$$\boldsymbol{B}^{(e)} = \boldsymbol{\nabla}\boldsymbol{N} \quad [\texttt{calc\_bdef\_sssdlt\_bstd}]$$
$$\Delta\boldsymbol{\varepsilon}^{(e)} = \boldsymbol{B}^{(e)}\ \Delta\boldsymbol{u}^{(e)} - \xi^{(e)}\left(\boldsymbol{\nabla}\varphi^h\right)^{(e)}\ [\![\boldsymbol{u}]\!]^{(e)}$$
$$\overline{\overline{\boldsymbol{\sigma}}}_{n+1}^{(e)} = \dot{\boldsymbol{\Sigma}}\left(\boldsymbol{\nabla}^s\boldsymbol{u}^{(e)} = \Delta\boldsymbol{\varepsilon}^{(e)}\right) \quad [\texttt{calc\_stress}]$$

(f) Calculate stress for regular gauss-points 1,2,3,4 (standard 2×2 gauss points for quadrilateral elements)

$$\boldsymbol{B}^{(e)} = \boldsymbol{\nabla}\boldsymbol{N} \quad [\texttt{calc\_bdef\_sssdlt\_bstd}]$$
$$\Delta\boldsymbol{\varepsilon}^{(e)} = \boldsymbol{B}^{(e)}\ \Delta\boldsymbol{u}^{(e)} - \xi^{(e)}\left(\boldsymbol{\nabla}\varphi^h\right)^{(e)}\ [\![\boldsymbol{u}]\!]^{(e)}$$
$$\boldsymbol{\sigma}_{n+1}^{(e)} = \dot{\boldsymbol{\Sigma}}\left(\boldsymbol{\nabla}^s\boldsymbol{u}^{(e)} = \Delta\boldsymbol{\varepsilon}^{(e)}\right) \quad [\texttt{calc\_stress}]$$

(g) Compute the increment of stress

$$\Delta\tilde{\boldsymbol{\sigma}}_{n+1}^{(e)} = \left(1-\xi^{(e)}\right)\left[\tau^{(e)}\left(\boldsymbol{\sigma}_{n+1}^{(e)} - \boldsymbol{\sigma}_n^{(e)}\right) + \left(1-\tau^{(e)}\right)\left(\overline{\boldsymbol{\sigma}}_{n+1}^{(e)} - \overline{\boldsymbol{\sigma}}_n^{(e)}\right)\right] +$$
$$+\ \xi^{(e)}\left(1-\gamma_{W\setminus SD}^{(e)}\right)\left[\left(\overline{\boldsymbol{\sigma}}_{n+1}^{(e)} - \overline{\boldsymbol{\sigma}}_n^{(e)}\right) + \gamma_{W\setminus SD}^{(e)}\left(\overline{\overline{\boldsymbol{\sigma}}}_{n+1}^{(e)} - \overline{\overline{\boldsymbol{\sigma}}}_n^{(e)}\right)\right]$$

(h) Compute the new stress

$$\tilde{\boldsymbol{\sigma}}_{n+1}^{(e)} = \tilde{\boldsymbol{\sigma}}_n^{(e)} + \Delta\tilde{\boldsymbol{\sigma}}_{n+1}^{(e)}$$

(i) Elemental internal forces vector

$$\boldsymbol{F}^{int(e)} = \sum_{gp=1}^{ngp} \boldsymbol{B}_{gp}^{(e)T} \left(\tilde{\boldsymbol{\sigma}}_{n+1}^{(e)} \right)_{gp} dV_{gp}^{(e)}$$

(j) Compute increment of different stresses

$$\Delta \overline{\overline{\boldsymbol{\sigma}}}_{n+1}^{(e)} = \overline{\overline{\boldsymbol{\sigma}}}_{n+1}^{(e)} - \overline{\overline{\boldsymbol{\sigma}}}_{n}^{(e)}$$
$$\Delta \overline{\boldsymbol{\sigma}}_{n+1}^{(e)} = \overline{\boldsymbol{\sigma}}_{n+1}^{(e)} - \overline{\boldsymbol{\sigma}}_{n}^{(e)}$$

(k) If the symmetric strong discontinuity formulation is used

$$\boldsymbol{r}^{(e)} = \boldsymbol{n}^{(e)T} \, \Delta \overline{\boldsymbol{\sigma}}_{n+1}^{(e)} \, de^{(e)} - \overline{\boldsymbol{\nabla} \varphi}^{(e)T} \, \Delta \overline{\overline{\boldsymbol{\sigma}}}_{n+1}^{(e)} * dV^{(e)}$$

else (if non-symmetric)

$$\boldsymbol{r}^{(e)} = \boldsymbol{n}^{(e)T} \, \Delta \overline{\boldsymbol{\sigma}}_{n+1}^{(e)} \, de^{(e)} - \frac{1}{l^{(e)}} \overline{\boldsymbol{\nabla} \varphi}^{(e)T} \, \Delta \overline{\overline{\boldsymbol{\sigma}}}_{n+1}^{(e)} * dV^{(e)}$$

(l) Compute residual

$$\boldsymbol{r}_{n+1}^{(e)k} = -\xi^{(e)} \boldsymbol{r}^{(e)}$$
$$||\boldsymbol{r}_{n+1}||^k = ||\boldsymbol{r}_{n+1}||^{k-1} + \sqrt{\left(\boldsymbol{r}_{n+1}^{(e)k} \right)^T \boldsymbol{r}_{n+1}^{(e)k}}$$

(m) Assemblage of internal force vector

$$\boldsymbol{F}_{n+1}^{int} = \underset{e \in \Omega}{\mathcal{A}} \left(\boldsymbol{F}^{int(e)} \right)$$

(n) Calculation of characteristic length

$$l^{(e)} = \left[\sum_{i=1}^{nc} \left(\frac{\partial N_i}{\partial x} \cos\theta + \frac{\partial N_i}{\partial y} \sin\theta \right) \phi_i \right]^{-1} \qquad [\texttt{le\_calc}]$$

(o) Compute the band width for Strong Discontinuity analysis

$$k_\infty = parak * l^{(e)} \quad [\texttt{input.dat >> PARAK = 0.01}]$$
$$h^{(e)} = \begin{cases} l^{(e)} & \forall q \leq q_{SD\,inj} \\ k_\infty - \left(k_\infty - l^{(e)} \right) \exp \left[A \frac{(q - q_{SD\,inj})}{(q - q_{k\infty})} \right] & \forall q_{SD\,inj} < q < q_\infty \\ k_\infty & \forall q \geq q_\infty \end{cases}$$

or for Weak Discontinuity analysis

$h^{(e)} = l^{(e)}$

(p) Write output elemental results [output_vector, output_scalar]

En loop over elements

2. Perform the double smoothing process to determine the crack path [smoth_var]

$$\boldsymbol{\psi} = \boldsymbol{M}_L^{-1} \underset{e\in\Omega}{\mathcal{A}} \left(\boldsymbol{M}^{(e)-1} \boldsymbol{M}_L^{(e)} \boldsymbol{\alpha}_n^{(e)} \right)$$
$$\boldsymbol{\mu} = \boldsymbol{M}_L^{-1} \underset{e\in\Omega}{\mathcal{A}} \left[\boldsymbol{M}^{(e)-1} \boldsymbol{M}_L^{(e)} \left(\frac{d\boldsymbol{\psi}}{d\boldsymbol{n}} \right)^{(e)} \right]$$

5.3 Subroutine le_calc

5.3.1 Description

Performs the double smooth procedure for the computation of the crack path.

5.3.2 Procedure

1. Choose vector normal to discontinuity $\boldsymbol{n}$

   IF $\boldsymbol{n}$ is to be chosen from to one more collinear to $\boldsymbol{v} = \nabla\boldsymbol{u}/||\nabla\boldsymbol{u}||$

   (a) Get the two normals to the discontinuity obtained from previous bifurcation analysis, and select one comparing with $\boldsymbol{v} = \nabla\boldsymbol{u}/||\nabla\boldsymbol{u}||$.

   $\boldsymbol{n}_1, \boldsymbol{n}_2 \leftarrow$ bifurcation()
   $d_1 = \boldsymbol{n}_1 \cdot \boldsymbol{v}$
   $d_2 = \boldsymbol{n}_2 \cdot \boldsymbol{v}$
   IF $d_1 > d_2 \Rightarrow \begin{cases} \boldsymbol{n} = \boldsymbol{n}_1 \\ \boldsymbol{m} = \boldsymbol{n}_2 \end{cases}$
   IF $d_1 < d_2 \Rightarrow \begin{cases} \boldsymbol{n} = \boldsymbol{n}_2 \\ \boldsymbol{m} = \boldsymbol{n}_1 \end{cases}$

   (b) Rotate the normal vector if needed, after comparing with a reference normal introduced by the user [input.dat >> NORMAL_REFERENCE NX = 0.70710678 NY = -0.70710678]

   $select = \boldsymbol{n} \cdot \boldsymbol{n}_{ref}$
   IF $select < 0 \Rightarrow \begin{cases} \boldsymbol{n} = -\boldsymbol{n} \\ \boldsymbol{m} = -\boldsymbol{m} \end{cases}$

   ELSE $\Rightarrow$ call $\boldsymbol{n}$ previously chosen as the one more collinear with $\boldsymbol{v} = \nabla\boldsymbol{\mu}/||\nabla\boldsymbol{\mu}||$ after double smoothing process [smoth_var] of the last time-step

2. Compute angle from normal components

$$\theta = \arctan\left(\frac{\boldsymbol{n}_x}{\boldsymbol{n}_y}\right)$$

3. Establish values of ϕ for each corner node according to their position with respect to the local axes

   IF $x_i' \geq 0 \;\Rightarrow\; \phi_i = 1$ ELSE $\phi_i = 0$

4. Calculate the characteristic length for the actual integration point

$$l^{(e)}(\xi,\eta) = \left[\sum_{i=1}^{nnode}\left(\frac{\partial N_i(\xi,\eta)}{\partial x}\cos\theta + \frac{\partial N_i(\xi,\eta)}{\partial y}\sin\theta\right)\phi_i\right]^{-1}$$

5. Compute vecrtor $\boldsymbol{v}$ to compare with $\boldsymbol{n}$ in the next time-step

$$\nabla\boldsymbol{u} = [\nabla N]\;\Delta\boldsymbol{u}$$
$$||\nabla\boldsymbol{u}|| = \sqrt{\nabla u(1,1)^2 + \nabla u(1,2)^2 + \nabla u(2,1)^2 + \nabla u(2,2)^2}$$
$$||\nabla\boldsymbol{u}||_x = \sqrt{\nabla u(1,1)^2 + \nabla u(1,2)^2}$$
$$||\nabla\boldsymbol{u}||_y = \sqrt{\nabla u(2,1)^2 + \nabla u(2,2)^2}$$
$$\boldsymbol{v} = \min\left(\frac{\nabla\boldsymbol{u}}{||\nabla\boldsymbol{u}||_x},\; \frac{\nabla\boldsymbol{u}}{||\nabla\boldsymbol{u}||_y}\right)$$

5.4 Subroutine `smoth_var`

5.4.1 Description

Performs the double smooth procedure for the computation of the crack path.

5.4.2 Procedure

1. Compute elemental mass matrix and assemble the global mass matrix

$$\boldsymbol{M} = \underset{e\in\Omega}{\mathcal{A}}\left(\int_{\Omega^{(e)}} \boldsymbol{N}^{(e)T}\,\boldsymbol{N}^{(e)}\,d\Omega\right)$$

2. Begin loop over elements to make the first smooth

   (a) Compute elemental mass matrices

$$\boldsymbol{M}^{(e)} = \int_{\Omega^{(e)}} \boldsymbol{N}^{(e)T}\,\boldsymbol{N}^{(e)}\,d\Omega$$

   (b) Calculate local smoothing variable at element nodes

$$\boldsymbol{\alpha}_{\boldsymbol{n}}^{(\boldsymbol{e})} = \int_{\Omega^{(e)}} \boldsymbol{N}^{(e)T} \boldsymbol{\alpha}^{(e)} \, d\Omega$$

(c) Assemble to calculate first smooth variable

$$\boldsymbol{\psi} = \boldsymbol{M}_L^{-1} \underset{e \in \Omega}{\mathcal{A}} \left(\boldsymbol{M}^{(e)-1} \boldsymbol{M}_L^{(e)} \boldsymbol{\alpha}_n^{(e)} \right)$$

End loop for first smooth variable

3. Begin loop over elements to compute derivatives and make the second smooth process

(a) Compute normal derivative of the first smooth variable make it the second variable to smooth

$$\left(\frac{d\boldsymbol{\psi}}{d\boldsymbol{n}} \right)^{(e)} = \left(\nabla \boldsymbol{N}^{(e)} \, \boldsymbol{\psi}^{(e)} \right) \boldsymbol{n}^{(e)}$$

(b) Compute elemental mass matrices

$$\boldsymbol{M}^{(e)} = \int_{\Omega^{(e)}} \boldsymbol{N}^{(e)T} \, \boldsymbol{N}^{(e)} \, d\Omega$$

(c) Assemble to calculate second smooth variable

$$\boldsymbol{\mu} = \boldsymbol{M}_L^{-1} \underset{e \in \Omega}{\mathcal{A}} \left[\boldsymbol{M}^{(e)-1} \boldsymbol{M}_L^{(e)} \left(\frac{d\boldsymbol{\psi}}{d\boldsymbol{n}} \right)^{(e)} \right]$$

End loop for second smoothing

4. Compute the function $\varphi^{(e)}$ which is going to take unit or null values for nodes belonging to Ω^+ and Ω^-, respectively. It is calculated searching for the sides crossed by the discontinuity. One can know which side is crossed looking for a change of sign in the variable $\boldsymbol{\mu}$ between the nodes that define the side.

IF $\quad \text{sign}\left(\mu_i^{side}\right) \neq \text{sign}\left(\mu_j^{side}\right) \Rightarrow$ side crossed

then, the function $\varphi^{(e)}$ may take values as

$$\varphi^{(e)} = \begin{cases} [0\,1\,0\,0] \\ [0\,0\,1\,0] \\ [1\,0\,1\,1] \\ [1\,1\,0\,1] \\ [0\,0\,0\,1] \\ \vdots \end{cases}$$

5. Calculate the gradient of the function

$$\nabla \boldsymbol{\varphi}^{(e)} = \nabla \boldsymbol{N}^{(e)T}\, \boldsymbol{\varphi}^{(e)}$$

6. Begin loop over elements to choose vector normal to discontinuity $\boldsymbol{n}$, only IF $\boldsymbol{n}$ is to be chosen from to one more collinear to $\boldsymbol{v} = \nabla\boldsymbol{\mu}/||\nabla\boldsymbol{\mu}||$

   (a) Compute the derivative of the smooth variable and the vector to select $\boldsymbol{n}$

$$\nabla \boldsymbol{\mu} = \nabla \boldsymbol{N}^{(e)T}\, \boldsymbol{\mu}$$
$$||\nabla \boldsymbol{\mu}|| = \sqrt{\nabla\boldsymbol{\mu}(1)^2 + \nabla\boldsymbol{\mu}(2)^2}$$
$$\boldsymbol{v} = \frac{\nabla \boldsymbol{\mu}}{||\nabla \boldsymbol{\mu}||}$$

   (b) Get the two normals to the discontinuity obtained from previous bifurcation analysis, and select one comparing with $\boldsymbol{v} = \nabla\boldsymbol{\mu}/||\nabla\boldsymbol{\mu}||$.

$$\boldsymbol{n}_1, \boldsymbol{n}_2 \leftarrow \texttt{bifurcation}()$$
$$d_1 = \boldsymbol{n}_1 \cdot \boldsymbol{v}$$
$$d_2 = \boldsymbol{n}_2 \cdot \boldsymbol{v}$$
$$\text{IF } d_1 > d_2 \Rightarrow \begin{cases} \boldsymbol{n} = \boldsymbol{n}_1 \\ \boldsymbol{m} = \boldsymbol{n}_2 \end{cases}$$
$$\text{IF } d_1 < d_2 \Rightarrow \begin{cases} \boldsymbol{n} = \boldsymbol{n}_2 \\ \boldsymbol{m} = \boldsymbol{n}_1 \end{cases}$$

   (c) Rotate the normal vector if needed, after comparing with a reference normal introduced by the user [`input.dat >> NORMAL_REFERENCE NX = 0.70710678 NY = -0.70710678`]

$$select = \boldsymbol{n} \cdot \boldsymbol{n}_{ref}$$
$$\text{IF } select < 0 \Rightarrow \begin{cases} \boldsymbol{n} = -\boldsymbol{n} \\ \boldsymbol{m} = -\boldsymbol{m} \end{cases}$$

   End loop over elements to choose $\boldsymbol{n}$

Appendix A

Interface subroutines

This chapter shows some subroutines of `commatfail` that serve as interfaces between general procedures and specific calculus. These interfaces are a comprehensible way to determine which specific procedure will be used. For example: the computation of stresses in a small strain and small deformation formulation can be different for each constitutive material model. Then, the interface `calc_stress_sssd` is used here to indicate the procedure to follow.

A.1 Interface `calc_stress`

A.1.1 Description

Chooses the next interface whether the problem is based on small strain and small displacement or not. As `commatfail` is still in a development stage, it has only the option for small strains and small displacements, but other formulations can be implemented.

A.1.2 Cases

Table A.1: Options in interface `calc_stress`

Case	Action
'SMALLSTRASMALLDISPLA'	CALL calc_stress_sssd
'SMALLSTRASMALLDISPLT'	CALL calc_stress_sssd
'SMALLSTRASMALLDISPLTBSTD'	CALL calc_stress_sssd
'SMALLSTRASMALLDISPLTBBAR'	CALL calc_stress_sssd
'SMALLSTRASMALLDISPLTWSDA'	CALL calc_stress_sssd

A.2 Interface `calc_stress_sssd`

A.2.1 Description

Call specific subroutines to calculate stress for small strains and small dispacements formulation.

A.2.2 Cases

Table A.2: Options in interface `calc_stress_sssd`

Case	Action
'ELASTIC'	CALL calc_stress_sssd_el
'ELASTOPLASTIC'	CALL calc_stress_sssd_elpl

Continue on next page

Table A.2 – continued from previous page

Case	Action
'ELASTOPLASTIC2'	CALL calc_stress_sssd_elpl2
'ELASTICDAMAGE'	CALL calc_stress_sssd_eldmg
'RANKINEMODEL'	CALL calc_stress_sssd_rankine
'RANKINEMODEL2'	CALL calc_stress_sssd_rankine2
'RANKINEMODEL3'	CALL calc_stress_sssd_rankine3_v3
'MATTEST'	CALL calc_stress_sssd_mattest

A.3 Interface e2dstd

A.3.1 Description

Choose the following interface of calls for specific tasks depending on the type of finite element.

A.3.2 Cases

Table A.3: Options in interface e2dstd

Case	Action
'RESTART_RD'	CALL rest_rd_e2dstd
'RESTART_WR'	CALL rest_wr_e2dstd
'CALCDOF'	CALL cdof_e2dstd
'CALC_FINT'	CALL cfint_e2dstd
'CALC_FEXT'	CALL cfext_e2dstd
'CALC_FDYN'	CALL cfdyn_e2dstd
'OUTPUT'	CALL wroutpost_e2dstd
'CALC_STIFF'	CALL stiff_e2dstd
'CALC_DYN_STIFF'	CALL stiff_dyn_e2dstd
'GET_REMESH_DATA'	CALL rmshedata_e2dstd
'TRANSF_REMESH_DATA'	CALL transfedata_e2dstd
'GET_LNODS'	CALL stdtrianmesh
	CALL getlnods_e2dstd
'GET_BOUND'	CALL getlnodb_e2dstd
'MESH_OUTPUT'	CALL wroutmsh_e2dstd
'SEARCH'	found = TRIM(lwcase(ename)) == TRIM(lwcase(eset%ename))
'ARRGESET'	CALL ini_e2dstd
'DELETE'	CALL del_e2dstd
'GET_ELEM_GEOMETRY'	CALL get_gtype_e2dstd
'GET_ELEM_TYPE'	strng = eset%etype
'GET_SECTION_TYPE'	CALL get_section_e2dstd
'GET_NAME_LIST'	CALL inc_vstg
'REMESH_CHECK'	EXIT
'CALC_EMASS'	CALL emass_e2dstd
'DENSITY_CHECK'	CALL denschk_e2dstd
'GET_NODE_LIST'	CALL get_nodelist
'GET_NGBR'	CALL get_ngbr
'wroutplot'	CALL wroutplot_e2dstd
'CONDS_RESID'	CALL conds_resid_e2dstd

Continue on next page

Table A.3 – continued from previous page

Case	Action
'ACT_CONDSVAR'	CALL act_condsvar_e2dstd
'PROD_CONDSVAR'	CALL prod_condsvar_e2dstd

A.4 Interface elemset

A.4.1 Description

Choose the following interface of calls for specific tasks depending on the type of finite element.

A.4.2 Cases

Table A.4: Options in interface elemset

Case	Action
elmtyp(1)='E2DSTD'	CALL e2dstd
elmtyp(2)='E3DSTD'	CALL e3dstd
elmtyp(3)='E2PFEM'	CALL e2dpfem
elmtyp(4)='E3PFEM'	CALL e3dpfem
elmtyp(5)='E2DMIX'	CALL e2dmix
elmtyp(6)='E2DMXD'	CALL e2dmxd

A.5 Interface calc_celas

A.5.1 Description

Choosses between two subroutines that calculate the constitutive tensor for linear elastic material, according to the type of problem to solve.

A.5.2 Cases

Table A.5: Options in interface calc_stress

Case	Action
'ELASTICLINEAR' → 'PLANESTRAIN'	CALL calc_isolin_celas
'ELASTICLINEAR' → 'PLANESTRESS'	CALL calc_isolin_celas_pstress

A.6 Interface stiff_e2dstd

A.6.1 Description

Call specific subroutines to calculate the stiffness matrix for element type E2DSTD, according to the formulation of the problem.

A.6.2 Cases

Table A.6: Options in interface `stiff_e2dstd`

Case	Action
'SMALLSTRASMALLDISPLA'	CALL stiff_e2dstd_sssdla
'SMALLSTRASMALLDISPLT'	CALL stiff_e2dstd_sssdlt
'SMALLSTRASMALLDISPLTBSTD'	CALL stiff_e2dstd_sssdlt_bstd
'SMALLSTRASMALLDISPLTBBAR'	CALL stiff_e2dstd_sssdlt_bstd
'SMALLSTRASMALLDISPLTWSDA'	CALL stiff_e2dstd_sssdlt_wsda

Appendix B

Variables

This chapter is for the users not used to the program variable saving system. It will help to know where is located each variable of the set of elements `e2dstd`.

B.1 Variables of the e2dstd set of elements

Variables for the hole set of elements of type `e2dstd`. This set of variables is stored in one variable of type `tp_e2dstd`.

Table B.1: Element set variables (`tp_e2dstd`)

Variable	Type	Description
`ename`	character	Set name
`etype`	character	Element type
`eform`	character	Formulation type
`qtype`	character	Quadrature type
`nelem`	integer	Number of elements
`nnode`	integer	Number of nodes/element
`ngaus`	integer	Number of Gauss points
`mgaus`	integer	Number of Gauss points for mass matrix
`lnods(:,:)`	real	Conectivities
`posgp(:,:)`	real	Gauss point coordinates
`posgpm(:,:)`	real	Gauss point coord. for mass matrix
`weigp(:)`	real	Gauss point weigths
`weigpm(:)`	real	Gauss point weigths for mass matrix
`nshape(:,:)`	real	Shape functions
`nshapem(:,:)`	real	Shape functions for mass matrix
`nderiv(:,:,:)`	real	Shape fun. derivatives
`nderivm(:,:,:)`	real	Shape fun. derivatives for mass matrix
`dmass(:,:)`	real	Mass integration point by element
`gv(:)`	`tp_e2dstd_gp`	Gauss point internal variables array
`ev(:)`	`tp_e2dstd_el`	Element variables
`next`	`tp_e2dstd`	Pointer to next set of elements

B.2 Gauss point variables

Gauss point internal variables are stored in variable `gv` of type `tp_e2dstd_gp`.

Table B.2: Gauss point internal variables (tp_e2dstd_gp)

Variable	Type	Description
gausv(:,:)	real	Internal las converged variables
tmpgv(:)	tp_rv	Temporal step increment variables
eout(:)	tp_out	Post-process data by integration point

B.3 Element variables

Element variables are stored in variable ev of type tp_e2dstd_el.

Table B.3: Element variables (tp_e2dstd_el)

Variable	Type	Description
sec	tp_sec	Section label by element
elmi(:)	integer	Integer variables by element
elmr(:)	real	Real variables by element
elmc(:)	real	Condensate variable by element
gout(:)	tp_gout	Post-process data by element

B.4 Section variables

Section variables are stored in variable sec of type tp_sec.

Table B.4: Section variables (tp_sec)

Variable	Type	Description
sname	character	Section user label
secnum	integer	Section number
stype	character	Section type
props(:)	real	Section properties
mat	tp_mat	Material data
next	tp_sec	Pointer to next section

B.5 Material variables

General material variables are stored in variable mat of type tp_mat.

Table B.5: Material variables (tp_mat)

Variable	Type	Description
mname	character	Material user label
matnum	integer	Material number
mtype	character	Material type
nsbmat	integer	Number of sub-material model
heads, lasts	tp_sbmat	List of submaterial models
next	tp_mat	Pointer to next material

B.6 Sub-Material variables

General sub-material variables are stored in variable `heads` and `lasts` of type `tp_sbmat`.

Table B.6: Sub-Material variables (`tp_sbmat`)

Variable	Type	Description
`sname`	character	Sub-Material user label
`stype`	character	Sub-Material type
`smodel(:)`	character	Sub-Material models
`props(:)`	real	Sub-Material real properties
`ncurve`	integer	Number of curves
`headc`, `lastc`	`tp_crv`	List of associated curves
`nsbmat`	integer	Number of sub-material level
`heads`, `lasts`	`tp_sbmat`	List of sub-material models inside sub-material
`next`	`tp_sbmat`	Pointer to next sub-material

B.7 Elemental real variables for elements of type `e2dstd`

Table B.7: Element real variables for `e2dstd` (`ev%elmr(:)`)

Variable	Type	Description
`elmr(1)`	$l^{(e)}$	Characteristic length of the element
`elmr(2)`	q_{bif}	
`elmr(3)`	$\boldsymbol{n}_1(x)$	Component x of the first vector $\boldsymbol{n}$ from bifurcation analysis
`elmr(4)`	$\boldsymbol{n}_1(y)$	Component y of the first vector $\boldsymbol{n}$ from bifurcation analysis
`elmr(5)`	$\boldsymbol{n}_2(x)$	Component x of the second vector $\boldsymbol{n}$ from bifurcation analysis
`elmr(6)`	$\boldsymbol{n}_1(y)$	Component y of the second vector $\boldsymbol{n}$ from bifurcation analysis
`elmr(7)`	$k^{(e)}$	Band width for Strong Discontinuity
`elmr(8)`	$\|\|\nabla \boldsymbol{u}\|\|$	Norm of the displacements gradient
`elmr(9)`	$\nabla \boldsymbol{u}(x)/\|\|\nabla \boldsymbol{u}_{xy}\|\|$	Normalized displacement gradient vector to select $\boldsymbol{n}$
`elmr(10)`	$\nabla \boldsymbol{u}(y)/\|\|\nabla \boldsymbol{u}_{xy}\|\|$	Normalized displacement gradient vector to select $\boldsymbol{n}$
`elmr(11)`	$de = dV(6)/l^{(e)}$	Used for integration in the internal force calculations
`elmr(12)`	$\boldsymbol{nn}_1(x)$	Component x of the vector $\boldsymbol{n}$ selected from $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$
`elmr(13)`	$\boldsymbol{nn}_1(y)$	Component y of the vector $\boldsymbol{n}$ selected from $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$
`elmr(14)`	$\boldsymbol{nm}_2(x)$	Component x of the vector perpendicular to $\boldsymbol{n}$ selected from $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$
`elmr(15)`	$\boldsymbol{nm}_1(y)$	Component y of the vector perpendicular to $\boldsymbol{n}$ selected from $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$
`elmr(16)`	q_{inj}	
`elmr(17)`	q_{sda}	
`elmr(18)`	qq	
`elmr(19)`	g_n	Internal variable to make the double smoothing process
`elmr(20)`	$\nabla\varphi(x)$	Component x of function φ gradient
`elmr(21)`	$\nabla\varphi(y)$	Component y of function φ gradient
`elmr(22)`		This field is not used for any variable
`elmr(23)`	GG	
`elmr(24)`	$\|\|\nabla \boldsymbol{\mu}\|\|$	Norm of the internal variable gradient
`elmr(25)`	$\nabla \boldsymbol{\mu}(x)/\|\|\nabla \boldsymbol{\mu}\|\|$	Component x of normalized internal variable gradient vector to select $\boldsymbol{n}$
`elmr(26)`	$\nabla \boldsymbol{\mu}(y)/\|\|\nabla \boldsymbol{\mu}\|\|$	Component y of normalized internal variable gradient vector to select $\boldsymbol{n}$

Bibliography

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